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Cover: Supercomputing in the field of materials science is the focus of this issue of *access*. Some applications in this discipline aid the R&D of more sophisticated microprocessors to drive compute engines. Creativity, which energizes this science, is represented by the butterfly—a time-honored symbol of the creative mind. Cover rendered in Adobe Photoshop on a Macintosh system; output to color separations on a Crosfield 646 scanner. (Concept and illustration, Carlton Bruett; technical support, Alan Schwenk; research, Fran Bond.)

access index

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1993 volume 7

1993 index

This document contains index entries for the 1993 *access* magazine. The three numbers used for the entries and subentries indicate the volume, issue, and page number(s) of the citation, in that order. For example, 7.2.6-7 means that the entry is in volume 7, issue 2, pages 6-7.

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MATERIALS SCIENCE RESEARCH AT NCSA

These prophetic words from Max Planck are especially meaningful today. His studies in atomic structure at the turn of this century began a revolution of innovative approaches that became known as the "new physics." In contemporary science—not just in physics—this thinking is no longer new because it is accepted practice. By now many generations are "familiar with it" indeed.

Almost a century since Planck took the first steps in quantum theory, high-performance computing is enabling great strides to be made in materials science research, whose practitioners base their numerical analyses in quantum theory. One of the most active areas of research at NCSA and the other NSF-sponsored HPCC centers, materials science is staging another kind of revolution with its researcher's findings.

Two distinguished, long-time materials science researchers—Arthur Freeman and David Pines—discuss their work (pages 8 and 13 respectively). David Ceperley explains his research into the fundamentals of condensed matter physics of the Quantum World (page 7). Using atomic-level simulations, Jim Adams and his research group are developing a variety of materials that have useful applications for consumers (page 16).

NCSA's Education Program is taking some new departures by examining classroom needs from the standpoint of students (page 23) and establishing an undergraduate internship program (page 25). Read about NCSA's newest partner, United Technologies Corp. (page 28). A recent book by a former NCSA employee is reviewed on page 29.

NCSA users are especially advised to check out changes underway with the CRAY-2 system (page 30) and the mass storage system (page 31). Other items of interest follow in the "center activities" section.

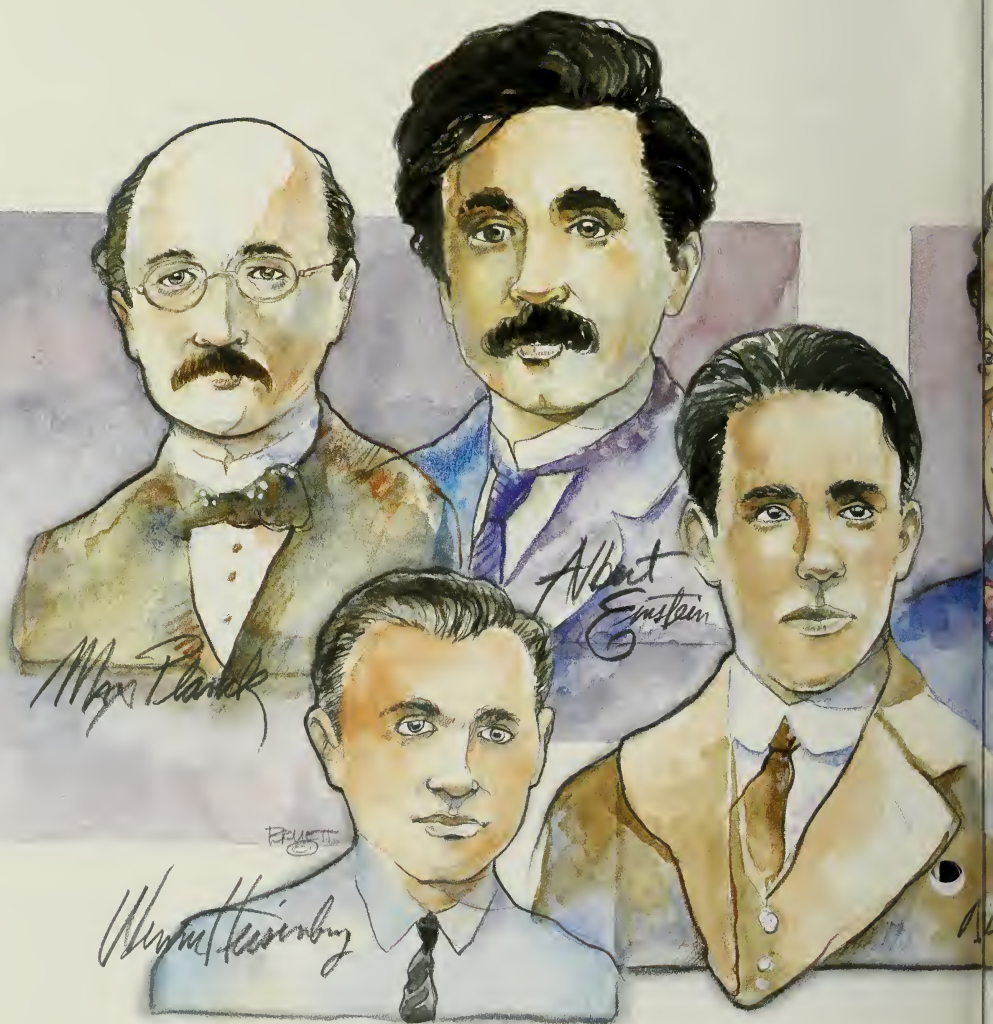
Beginning with this issue of *access*, we have a different look for enhanced readability and better integration of articles, especially in the departments.—*Fran Bond, Editor*

"A new scientific truth does not triumph by convincing its opponents, but rather because its opponents die, and a new generation grows up that is familiar with it."

— Max Planck (1858–1947)



What *is* Matter



als Science?

by Fran Bond, Publications Editor; Illustration by Carlton Bruett



Exploring known materials or enhancing their atomic structure to give them new properties is the work of materials scientists. This might be called the “growth” field of science because of its rapid advancements in R&D. It is considered by many to be a critical area for the future of our society.

A product of this discipline—Intel’s 486 computer chip—provoked one of the most energetic upsurges in the stock market in recent memory during the winter of 1993. The chip’s proficiency can be attributed to designers working closely with researchers in materials science. Yet today’s 0.5-micron sized electronic components will be replaced with even smaller ones in the future—increasing the challenges facing materials scientists and engineers.

Tougher plastics, solutions to crack-formation in ceramics and metals, and better lubricants are some other results of materials science research. Sweden’s clean, energy efficient levitating trains are another. Worldwide usage of such transportation could grow out of refinements in present day materials research.



Understanding the electronic structure of quantum materials requires intensive number crunching. The complexity of the resulting mathematics intrinsic to the discipline assures that high-performance computers and computational science are the primary tools of materials science. Knowledge base of the field is interdisciplinary—dovetailing chemistry, physics, and some aspects of engineering. Research, development, and productization are interconnected—

Materials Science continued on page 6

seemingly more so than in other fields.

Researchers use the fundamental laws of quantum mechanics to predict the physical and chemical properties of elements and compounds. Developers and designers use computer simulations for modeling rather than traditional hands-on methods.



The theoretical foundation of materials science, quantum physics, emerged over the first quarter of this century when it became evident that the classical mechanics of Newtonian physics could not explain atomic structure. Deterministic theories—accepted for centuries—broke down when they were used to explain the strange behaviors of subatomic particles, x-rays, and similar elements of emerging scientific inquiry. Their attributes, or properties, defy traditional thought and solutions.

In 1900 the search for an answer to the quixotics of atomic structure began when German physicist Max Planck proposed that electromagnetic radiation comes in small bursts (or *quanta*) of energy. Five years later Albert Einstein postulated the photoelectric effect, which by 1916 was accepted in the growing experimentalist community. This discovery won him the Noble Prize in Physics in 1921.



Many other now-famous European physicists contributed to the theories of what came to be called the “new physics” (see illustration, page 4).

Using the model of the simplest atom, hydrogen, Neils Bohr (1913) formed the theory of atomic structure and developed what is sometimes referred to as the “Copenhagen interpretation of quantum mechanics.” Werner Heisenberg, famous for his uncertainty principle of 1927, formulated what he called “matrix mechanics” (1925), and Erwin Schrödinger wrote the basic equation of electronic structure (1926). These were major, almost simultaneous breakthroughs in quantum theory. Schrödinger’s equation still stands as the mathematical foundation of materials science.

“It has been an outstandingly successful theory and underlies nearly all of modern science and technology.”

—Stephen Hawking



Quantum mechanics brought the concepts of unpredictability, randomness, and probability into science at a fundamental level with these discoveries. The idea of duality—waves as particles, particles as waves—was part of this thought. At about the same time in many other fields—philosophy, literature, and the arts, to name a few—new ideas were dramatically replacing traditional concepts.

Stephen Hawking summarizes what went on in science: “The theory of quantum mechanics is based on an entirely new type of mathematics that no longer describes the real world in terms of particles and waves; it is only the *observations* of the world that may be described in those terms. There is thus a duality between waves and particles in quantum mechanics: for some purposes it is helpful to think of particles as waves and for other purposes it is better to think of waves as particles.” According to Hawking—and countless others concur—“it has been an outstandingly successful theory and underlies nearly all of modern science and technology.”



Today quantum theory governs the basics of chemistry, biology, and the physics that drives the development of essential electronic components as well as most physical sciences.

In contemporary computational science, activity in applying the laws and theories of quantum mechanics seemingly is almost as vigorous as was the earlier search for its explanation. Twelve percent of NCSA’s current users are materials scientists (see page 19). Many of the problems materials scientists explore are listed among the Grand Challenges of computational research.



This research energy was jokingly likened to athletics by a scientist who equated the search in his area of expertise to that of a “sporting event”—given a sudden growth in papers and meeting attendance. News of this competitive spirit even reaches the popular press—in the race for a better superconductor, for example.

As consumers, we may profit from today’s scientific discoveries by using seemingly “twenty-first century” products that spin off from materials science research. It remains to be seen if superconducting levitating trains will run on time.

NOTE: Randall Graham contributed to this article.

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Seeing into the Quantum World

by Randall Graham, Science Writer

"I work at the fundamental level trying to solve the original equations of quantum theory to build from the ground level an understanding of atomic structure," says UIUC Physics Professor and NCSA Research Scientist David Ceperley. "A lot of the work I do is not really materials science, but the same mathematical problem." Ceperley's goal is to advance the field of materials science by developing computational techniques that can be applied broadly to many types of systems where quantum effects are important.

Over the years Ceperley has been working on methods to directly simulate the properties of hydrogen and helium. In one sense, these atoms are simple—having few electrons. In another sense, their behavior is especially complex since both their electrons and nuclei exhibit quantum motion—a property not found in heavier atoms.

"Hydrogen and helium are a little difficult to work with," says Ceperley, "because the nuclei of these atoms are light; hence, they move around a lot. Most computational methods treat these nuclei simply as classical particles that do not have quantum motion."

QMC techniques

Quantum Monte Carlo (QMC) methods—algorithms that use statistical sampling to solve the Schrödinger equation—are what Ceperley relies on. Quantum particles cannot have both their velocity and location measured at the same time, so scientists represent the particles as waves of probability—the probability that particles will be in a given location at any given time.

Ceperley sets simulated electrons into random motion based directly on the Schrödinger equation. In hydro-



"We won't exhaust this science for centuries."

—David Ceperley

gen and helium, both electrons and nuclei are set in motion. Next Ceperley takes many computational "snapshots" of his particles. By superimposing the results, a picture of average behavior begins to take shape.

QMC studies

Together with UIUC Physics Professor Richard Martin, Ceperley leads a 15-member group of postdoctoral research associates, visitors, and graduate students in theoretical condensed matter physics—a field which studies solids, liquids, and gases. QMC studies by the Ceperley-Martin group have revealed the behavior of helium atoms near the transition temperature where helium changes from an ordinary

fluid to a superfluid. These calculations are of interest to Ceperley and Martin's colleagues in the UIUC Center for High-Temperature Superconductivity, of which they are associate members.

Similar computational methods allowed Ceperley and Berni Alder of Lawrence Livermore National Laboratory to calculate the arrangement of atoms in bulk hydrogen subjected to extremely high pressure and its transition from insulator to metal. Recently UIUC graduate student Vincent Natolie, Martin, and Ceperley predicted that hydrogen, at 3 Mbars (megabars), should form a crystal lattice similar to diamond.

These efforts require expanded computing power. For example, Werner Krauth, former NCSA postdoctoral research associate of Ceperley (now at the Ecole Normale Supérieure, Paris), pioneered the use of clustered workstations at NCSA. Krauth utilized the equivalent of

Quantum World continued on page 20

Manipulating

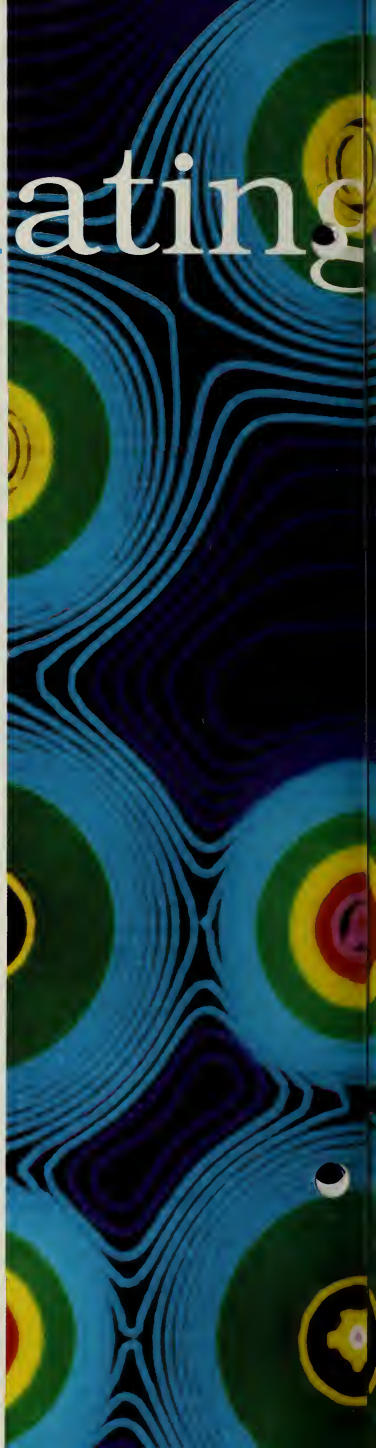
Medieval alchemists dreamed of transmuting common base metals into gold—such miraculous conversions proved impossible, of course. Today, thanks to discoveries in the fields of computational physics and computational chemistry, researchers are making startling progress in understanding and manipulating matter at the atomic and molecular level.

While no one yet has figured out how to turn lead into gold, advances made possible by high-performance computing (HPC) have enabled scientists to use the elements provided by nature to create entirely new artificial materials with properties tuned to meet a variety of mankind's needs. A premier example can be seen in the work of Arthur J. Freeman, NCSA principal investigator and Morrison Professor of Physics at Northwestern University.

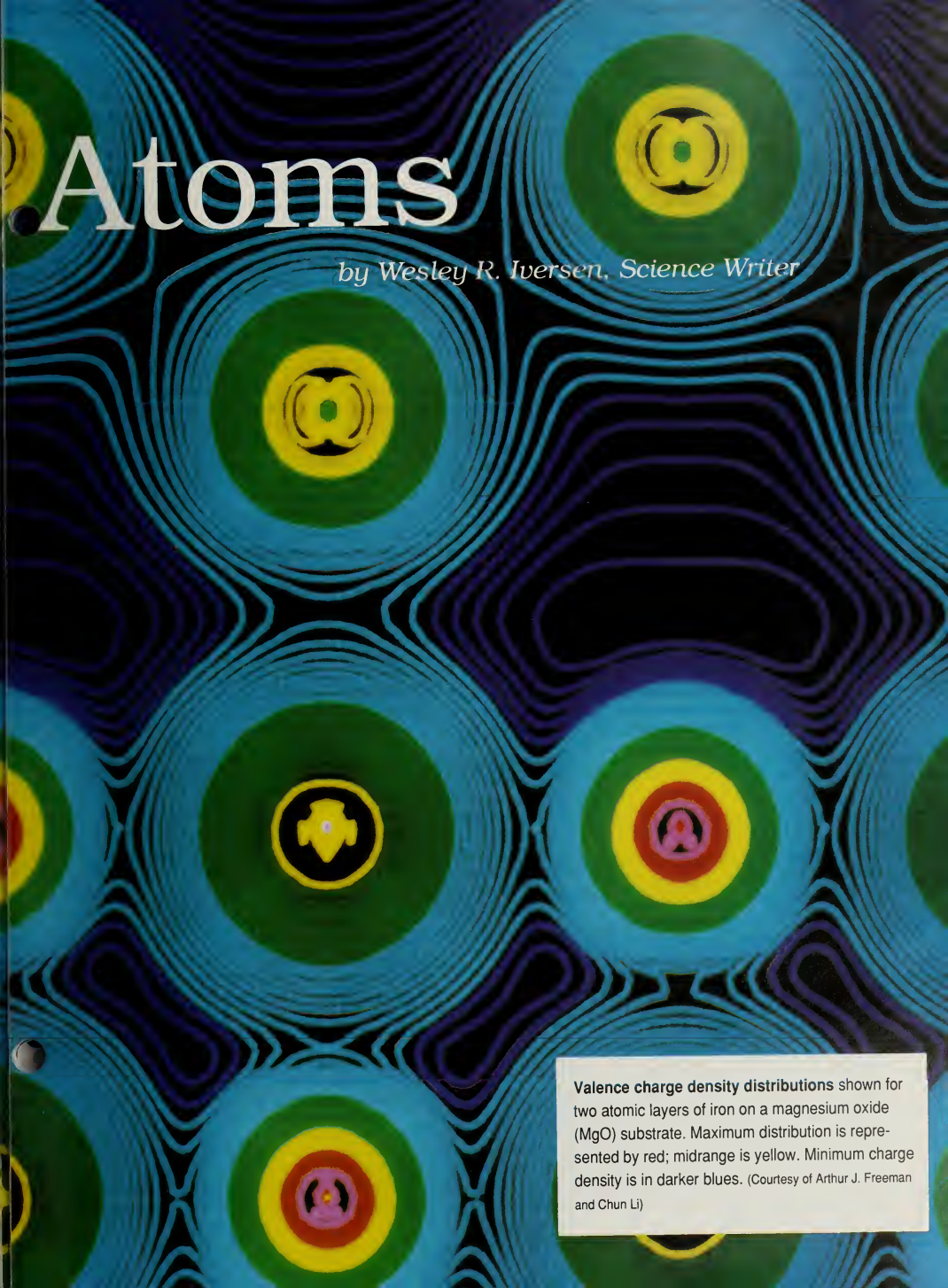
Fine tuning materials

Over the past several years, Freeman's groundbreaking theoretical research using Cray supercomputers at NCSA and elsewhere has earned international acclaim. Today he is recognized as one of the pioneers of computational physics. The work of Freeman and his associates is influencing the direction of artificial materials research and is expected to have major impact in areas such as magnetic memories and recording, semiconductors, and superconducting materials.

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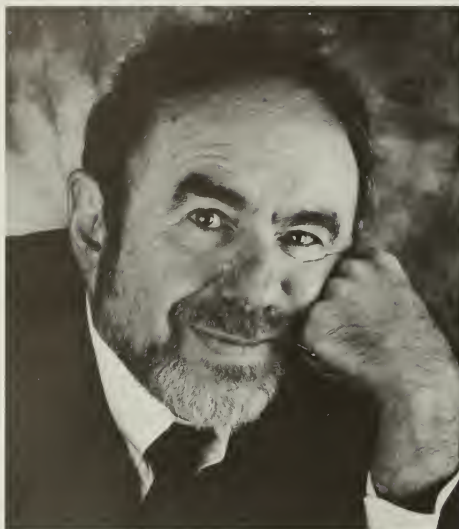


Atoms



by Wesley R. Iversen, Science Writer

Valence charge density distributions shown for two atomic layers of iron on a magnesium oxide (MgO) substrate. Maximum distribution is represented by red; midrange is yellow. Minimum charge density is in darker blues. (Courtesy of Arthur J. Freeman and Chun Li)



"Mankind is no longer restricted to relying on nature to provide us with materials."

—Arthur J. Freeman

Manipulating atoms continued from page 8

He is also doing additional research on other types of materials, such as aluminum intermetallics used in the aerospace industry.

The Northwestern professor is quick to point out that the opportunities for computational physics research are "as broad as they are deep. We deal with all kinds of materials, without restriction. Ultimately, we hope that new understanding of all of these materials will be transferred to making new materials with properties that [mankind] can use."

HPC simplifies solutions

Using quantum theory and the laws of quantum mechanics, which govern the motion and interactions of electrons and nuclei in all materials, it is theoretically possible to determine all of the properties of matter—electromagnetic, thermal, mechanical, and chemical—Freeman explains.

Due to the enormity and complexity of the calculations involved, quantum theory defies direct solution. For example, a direct calculation to determine electron orbitals in a solid would require solving a large set of differential equations for each orbital of around 10^{23} electrons in the material. As a result, various methods based on approximations are required that can reduce the number of equations, but they can also throw doubt on the results.

Today's supercomputers, capable of billions of calculations per second, have opened a new frontier. According to Freeman, computational physicists can now solve electronic structure theory problems to much higher degrees of precision, thanks to these machines. They are also able to tackle problems 100 to 1,000 times more complex than those previously considered.

"The ability to do calculations and simulations rapidly has meant, for us, a revolution," he relates. "Over the years, methods such as the density functional theory of Hohenberg, Kohn, and Sham [1964–65] have evolved and developed. It's only because of access to supercomputers that we have been able to do calculations without approximations, other than the local density approximation inherent in current applications of the method."

FLAPW approach to magnetism

Much of Freeman's current work relies on a technique known as the full potential linearized plane wave (FLAPW) method—developed in 1980 by Freeman and postdoctoral associates Henry Krakauer and Erich Wimmer and graduate student Michael Weinert.

Based on a local density functional theory approach, the FLAPW method provides a highly precise method for calculating the electronic structure and properties of materials. FLAPW's key feature is its ability to solve the Poisson equation in 3D. (The Poisson equation relates the electrostatic potential of a material to its electron distribution.) Despite the fact that the potential acting on electrons is 3D, previous solutions were limited to a 1D potential to make the calculations manageable.

Freeman and associates have invested about 18 person-years in the development of FLAPW codes for Cray supercomputers. Initial work with the code was done at Lawrence Livermore National Laboratory; enhanced versions are used at NCSA and elsewhere by Freeman and a growing research community.

Using FLAPW, Freeman and associates have made some innovative discoveries. In the early 1980s, they predicted that the level of magnetism seen in common magnetic materials would be much greater at the surface than in the bulk of the material. In iron, for instance, the so-called magnetic moment of surface layer atoms was predicted to be 2.98 Bohr magnetons—about 40% higher than that measured in bulk atoms. In chromium, the difference is even more dramatic: at 2.5 Bohr magnetons at the surface versus 0.6 Bohr magnetons in the bulk. These predictions were confirmed by experiments at the University of California at Berkeley.

Through FLAPW simulations, the Northwestern researchers discovered that magnetism can be even further enhanced when materials are formed into single atomic layers. They found that the deposition of such monolayers onto certain other materials does not significantly decrease the effect. A monolayer of chromium deposited on gold, for example, produces a magnetic moment of 3.7 Bohr magnetons. "So now you're up to six times larger than what the chromium moment is in the bulk," Freeman says. "That's truly a giant moment."

Recent predictions by Freeman and others show that elements that are not magnetic in their natural state can be made to exhibit magnetism when deposited in monolayer form on a substrate.

"Vanadium, which is just to the left of chromium in the periodic table, is not magnetic—either in bulk or at the surface. But if you put a layer of vanadium onto silver, it becomes magnetic with a sizeable magnetic moment. So here, we've made magnetism in a material that's never been magnetic before. For the other materials, we've enhanced the magnetism dramatically—40% for iron and 300% for chromium on the surface. For chromium on gold, the increase is 500%."

Though still theoretical, these discoveries take on increasing importance given the wider availability of advanced equipment such as molecular beam epitaxy (MBE) systems that can be used to synthesize actual physical samples of monolayers (on benign substrates) that were first simulated on a supercomputer. "These beautiful machines represent a new frontier which is driving the field of artificial materials," Freeman notes.

Exploring other electrical properties

"Mankind is no longer restricted to relying on nature to provide us with materials. We can make our own," says Freeman. "We can make new and exotic materials—or materials that have properties that avoid the complexities of materials that you buy off the shelf. This is what the revolution is all about."

Beyond magnetic properties, the electrical characteristics of monolayers and ultrathin films are also of great import, particularly in the semiconductor industry. In other work with the FLAPW code, Freeman is simulating mechanisms found at the so-called heterojunctions formed in advanced electronic circuits at the interface of two materials. He is also studying the unusual properties of *superlattices*—sandwich-like materials made by alternating layers of metallic, semiconducting and/or insulating elements.

Worldwide interest

Spurred by the discoveries of Freeman and others, worldwide scientific interest has been growing by leaps and bounds. For example, a variety of national and international conferences are now devoted exclusively to monolayer magnetism and other fields related to artificial materials theory and practices.

Another "hot" field is that of high-temperature superconductors. Early in 1987, Freeman and his collaborators were among the first to use supercomputers to investigate the properties of a newly discovered class of these materials consisting of complex yttrium-barium-copper-oxide compounds. (See simulation, page 12.) These new superconductors (so-named because of their ability to conduct electricity with no resistance, while generating strong magnetic fields) operate at temperatures much higher than previously thought possible. As such, they hold potential for revolutionary advances in computers, electric motors, and magnetically levitated trains.

Professor Arthur J. Freeman
(left) and Northwestern student Stefan bei der Kellen work at an Apollo terminal linked to NCSA's supercomputers. (Courtesy of Northwestern University)



Manipulating atoms continued on page 12



Vertical slice showing valence charge density distributions of copper and oxygen atoms in a yttrium-barium-copper-oxide superconductor— $\text{YBa}_2\text{Cu}_3\text{O}_x$. Highest density is red; lowest density is deep blue. The all-red atoms are oxygen; those with blue centers are copper.

(Courtesy of Arthur J. Freeman, Sandro Massidda, and Jaejun Yu)

When copper-oxide materials were first discovered, researchers around the world proposed a variety of complex theories to explain high-temperature superconductivity. Through FLAPW simulations of the new materials, Freeman and his group were able to make predictions which were later proved out in laboratory experiments by others.

"I'm happy to say that of all the theories that were proposed about the normal state, the only theory that still survives is electronic structure theory," Freeman says. "Thanks to supercomputers, we were able to respond quickly to the 1986 Nobel Prize-winning discoveries of Bednorz and Müller and later Chu and collaborators [of high-temperature superconductors] and to investigate the most complex materials we had ever come across. We showed how the crystallographic structure, the chemical and physical properties, and the electronic structure are related."

Code development

While Freeman makes use of the basic scientific library software provided at NCSA, all of his heavy computing done on the center's CRAY-2 and CRAY Y-MP systems uses FLAPW and other codes developed by the Northwestern group. "To know a code intimately, you have to write it," Freeman notes. "One major software package that we have developed, called DMol, has now become a commercial code." The DMol package, based on local density functional theory for the study of molecules, clusters, and aggregates, is available from BIOSYM Technologies Inc., San Diego, CA.

Given the complexity of his research, it is not surprising that Freeman is one of NCSA's major NSF-supported users. He is also a major user at the Pittsburgh Supercomputing Center. The Northwestern group is constantly working to make their codes run more efficiently on the Crays and is working on enhancements which will "allow us to do a better job with many-body problems." They plan to "parallelize" FLAPW for use on the Thinking Machines' CM-5, NCSA's massively parallel processing machine.

Rewarding style of work

For his work in monolayer magnetism, in late 1990 Freeman received the first Materials Research Society Medal. In September 1991, at a ceremony held in Edinburgh, Scotland, the International Union of Pure and Applied Physics (IUPAP) presented him with its first Award in Magnetism [see *access*, September–December 1991].

On bestowing the award, Russian academician S. A. Vonsovsky cited the "intensity" of Freeman's work in "hot" fields and utilization of "novel computational techniques." In 1992 Freeman was elected to the Academy of Natural Sciences of Russia and the Russian Academy of Sciences (formerly the Soviet Academy of Sciences).

"When people ask me why I'm so enthusiastic and why I still work so hard, it's because of the opportunity to do what we couldn't dream about, even a few years ago—the advances having been so enormous and so exciting," Freeman says. "The sky is really the limit." ▲

Understanding high-temperature superconductivity

by Jarrett Cohen, Staff Associate, Director's Office

"Superconductivity is perhaps the most remarkable physical property in the universe," says David Pines, UIUC Center for Advanced Study Professor of physics and electrical and computer engineering, who has been seeking to understand superconductivity for nearly 40 years. Pines' research in physics ranges from microscopic processes to neutron stars.

"What makes superconductors so fascinating is their ability to carry electrical current without resistance and to shield out external magnetic fields," he adds.

Discovered in 1911, little progress was made in developing a fundamental theory of their behavior until the 1957 publication of the microscopic theory, or BCS theory, by John Bardeen, Leon N. Cooper, and J. Robert Schrieffer, for which they were awarded the Nobel Prize in Physics in 1972. The BCS theory describes superconductivity in low-temperature metals—such as mercury and lead—and is based on an attractive interaction between electrons that results from their coupling to phonons.

Phonons are quantized modes of atomic vibration that propagate throughout the lattice of a solid. In low-temperature superconductors, *quasiparticles* (electrons plus their associated screening clouds) disturb the phonons and create a force that overcomes the electrons' repulsive charges. The electrons then form a quantum state made up of Cooper pairs, which cannot scatter off the phonons, thereby eliminating resistance.

Until recently, essentially all superconductors were stable only at exceedingly low temperatures (typically 15 Kelvin, or -258° Celsius). Any devices that incorporated them had to be cooled with liquid helium (4.2K), which costs \$10 per gallon, and had to be handled by Ph.D.-level technicians. Factors like these have made using these low-temperature superconductors very expensive for commercial applications.

Despite these difficulties, practical uses have resulted, including magnets, such as those in magnetic resonance imaging devices, and SQUIDS (Superconducting Quantum Interference Devices), which are capable of detecting minute magnetic fields.

High-temperature superconductors

Matters changed dramatically in 1986 when the first high-temperature superconductor was discovered by K. Alex Müller and J. Georg Bednorz at the IBM Research Laboratory in Zürich, Switzerland. This ceramic compound of lanthanum, barium, copper, and oxygen ($\text{La}_{2-x}\text{Ba}_x\text{CuO}_4$) becomes a superconductor at 35K.



"Superconductivity is perhaps the most remarkable physical property in the universe."

—David Pines



Another team soon found superconductivity in a related material, an yttrium-barium-copper-oxygen compound ($\text{YBa}_2\text{Cu}_3\text{O}_7$), at 90K, well above the temperature at which nitrogen liquefies.

"A clear indication of the importance attached to the discovery of these new superconducting materials is that Müller and Bednorz were awarded the Nobel Prize [in Physics] within a year of making it—about the fastest turnaround I have seen," Pines says.

With liquid nitrogen 50 times cheaper than helium and thus the promise of commercial viability for the new materials, Pines says that a scramble—involving venture capitalists as well as scientists and engineers—ensued to find new high-temperature superconductors and the reason why they superconduct at such high temperatures.

Condensed matter physicists were particularly caught up in the race. Pines cites a special session of the 1987 American Physical Society meeting—the "Woodstock of physics," it has been called—for which 4,000 people showed up; that was 2,000 more than the hall could hold!

"Despite the intensive efforts of the theoretical physics community and some 5,000 papers later," Pines says, "there is still no clear consensus on the answers to three fundamental questions about the new superconductors." He considers these to be: What is the nature of the normal state? What is the character of the superconducting state? What is the physical origin of their superconductivity?

*"We need more memory . . .
to go down to lower
temperatures and look
at all the properties in the
superconducting state."*

—Philippe Monthoux

A new theory

In his attempt to answer these questions, Pines drew upon his long and close collaboration with Bardeen on superconductivity and related low-temperature phenomena. Pines worked as Bardeen's first postdoctoral associate in superconductivity (1952-55) before joining the Princeton University faculty. The BCS group built on electron-phonon interaction work in which he played a leading role.

"What I learned from Bardeen is a 'bottom-up' approach to scientific research," Pines says. "You have to first follow the experiment closely, especially when dealing with a major unsolved problem. Second, you should try to keep as open a mind as possible, looking at several possible avenues before fixing upon one when you're close to finding the answer."

Taking Bardeen's philosophy to heart when structuring his research program on high-temperature superconductivity, Pines began with evidence from nuclear magnetic resonance (NMR) experiments carried out by Physicist Charles Slichter's UIUC research team.

"These show that the magnetic behavior of the new superconductors is quite bizarre," Pines says, so much so that he decided that the magnetic interaction between the electrons in these systems must be playing a key role.

"The basic cause of the magnetic interaction is associated with the fact that electrons have a spin [either up or down] and therefore are capable of interacting magnetically through their spins," Pines says. "In . . . high-temperature superconductors, this magnetic interaction between the electrons can be very strong, changing their normal state behavior and causing the superconducting transition."

"It gives rise not to the usual kind of superconductivity . . . , in which the fundamental interaction is attractive," he continues. "But rather this spin-fluctuation-induced interaction is repulsive for the usual BCS pairs but becomes attractive when one looks at quite subtle effects associated with the relative angular momentum of the pairs of electrons involved."

Supercomputer analysis

Spin-fluctuation-induced superconductivity was not a completely new idea. After the 1986 discovery, "many people went in this direction at first but got quickly discouraged," Pines says. "Each of their reasons for getting discouraged has turned out to be wrong."

"It is enormously important to start out with the right model Hamiltonian for the low-energy properties and then to solve accurately the equations that describe the superconducting transition and the normal state properties, taking into account completely the structure of the magnetic interaction in momentum and frequency space," he says. "You can only do this in a reasonable period of time with a supercomputer. . . ."

"If you get an approximate solution, you find that you get completely the wrong answer," Pines adds. "This is one reason why people had not pursued this approach—they couldn't get reasonable quantitative results by following the usual path, making the approximations that were valid for ordinary superconductors."

Even on a supercomputer, Pines says that carrying out the solution of the Eliashberg equations, which describe the strong coupling effects associated with the spin fluctuations, to the needed degree of accuracy requires a state-of-the-art approach. Philippe Monthoux, then a graduate student in physics at UIUC (and now a postdoc at the Institute for Theoretical Physics, University of California at Santa Barbara), recognized that Fast Fourier Transforms (FFT) would enable accurate solution on NCSA's CRAY Y-MP system. He carried out the calculations in the spring and summer of 1992.

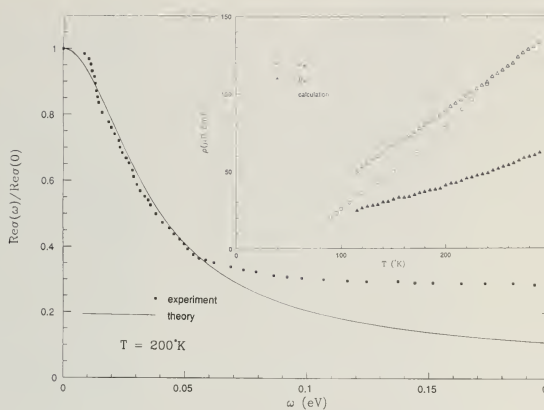
Monthoux says the problem is two-dimensional, with two momentum directions and one "imaginary" time dimension. Momenta are described by a 64 x 64 lattice that can have anywhere from 100 to 640 frequencies. The frequencies depend on the temperature, with their number increasing as the system's temperature lowers to the superconducting transition.

According to Monthoux, modeling these frequencies in particular pushes the Cray system's memory limits, with 16 Mwords consumed for most of the runs and 32 Mwords at 640 frequencies. These calculations took in all approximately 150 hours of Cray time.

Properties explained

Through computational experiments on $\text{YBa}_2\text{Cu}_3\text{O}_7$, a 90K superconductor, using input parameters for their model taken from NMR and other studies, Monthoux and Pines gained a number of insights into the compound's properties, which they incorporated into the general theory.

Regarding its normal state, they discovered that the compound is a quite new state of matter, which they call "a nearly antiferromagnetic Fermi liquid." "These systems are failed antiferromagnets, in which neighboring spins

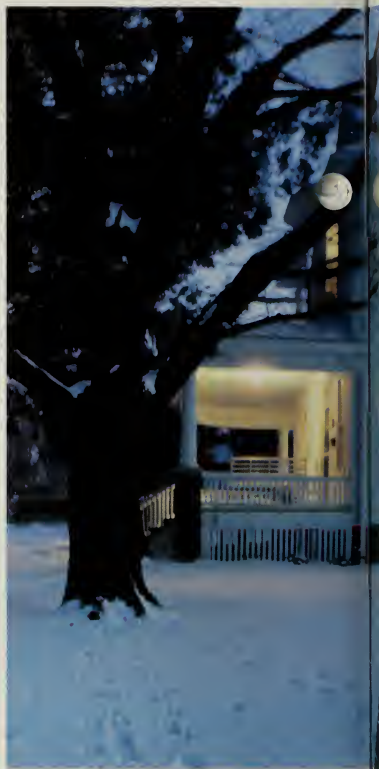


The calculated frequency dependence of the optical conductivity $\sigma(\omega)$ for the high-temperature superconductor $\text{YBa}_2\text{Cu}_3\text{O}_7$ is compared with the experimental result at a temperature of 200K. At high frequencies there are contributions to $\sigma(\omega)$ which are not included in the model. The inset shows the calculated resistivity, $\rho(T)$, for an electric field oriented in the copper-oxygen planes; it is compared with the experimental result of D. M. Ginsberg's group (UIUC) for ρ_a and ρ_b , the resistivities in the a and b directions. The simplified model does not distinguish the a and b (i.e., x and y) directions. In all of these calculations, the coupling constant between quasiparticles and spin fluctuations was chosen such that the transition temperature to the superconducting state is the experimental value of 90K. (Courtesy of David Pines)

BY SARA LATTA, SCIENCE WRITER

PHOTOGRAPH BY THOMPSON-McCLELLAN PHOTOGRAPHY

Better paints, adhesives, coatings, and automobile engines plus more efficient production of electricity—for the home and industry—is available via materials science.



ATOMIC-LEVEL COMPUTER SIMULATIONS IN MATERIALS SCIENCE

What do improved automobile catalytic converters, more efficient solar cells, stronger machine tools, and better adhesives have in common? They are all among the target applications for the pioneering atomic level computer simulations carried out on NCSA's CRAY Y-MP system by Jim Adams, UIUC assistant professor in materials science engineering.

The unifying thread running through the work in Adams' group of six graduate students and three postdoctoral fellows is the fact that little atomic-level simulation has been done on any of his project areas.

From diamonds to polymers

One of Adams' projects focuses on diamond film growth—the deposition of a very thin film of carbon atoms in the characteristic crystalline structure of diamond through a process called chemical vapor deposition, or CVD. There are a couple of possible



applications for diamond films, according to Adams. "Diamond films might be a very good way to make much harder coatings for materials. Machine tools coated with a diamond film would last a lot longer," says Adams. "And, because diamond is also the world's best heat conductor, diamond films could have important applications in microelectronics." The arrangement of atoms on the surface of diamond films has been impossible to determine experimentally. According to Adams, "We've done the first realistic calculations of the structure of the diamond surface."

Amorphous silicon thin films—also manufactured by a CVD process—are the primary component of those solar cells that power calculators and a host of other devices. Although amorphous silicon (so-called because of the random, rather than crystalline,

arrangement of the silicon atoms) is quite inexpensive, it is only about 10% efficient in converting sunlight into electricity. Unfortunately, according to Adams, that efficiency drops to 8% when the material is exposed to sunlight for 24 hours—effectively a 20% decrease in efficiency.

"We're really the first group to determine the atomic defects in amorphous silicon that cause this degradation in efficiency," says Adams. "We'd like to prevent that. Solar cells produce electricity for only slightly more than the cost of present-day nuclear power reactor," he continues, "and the price keeps going down. It's possible that we could cover substantial areas of the desert with solar cells, for example, and supply most of the electricity for the U.S."

Adams is also using atomic-level simulations to investigate the adhesion of polymers to different types of surfaces, including metals and metal oxides. "Polymers, in general, don't stick very well to other materials," says Adams. By simulating the addition of different types of side groups to the polymers, Adams determines the modifications that help polymers form stronger bonds with the substrate—without otherwise affecting the properties of the polymer. "We hope that these studies can contribute to everything from stronger adhesives to better paints and coatings," says Adams. Perhaps not surprisingly, Adams' group is the first to study the atomic-level bonding of functional groups in polymers to metals, metal oxides, and semiconductors.

Catalytic properties

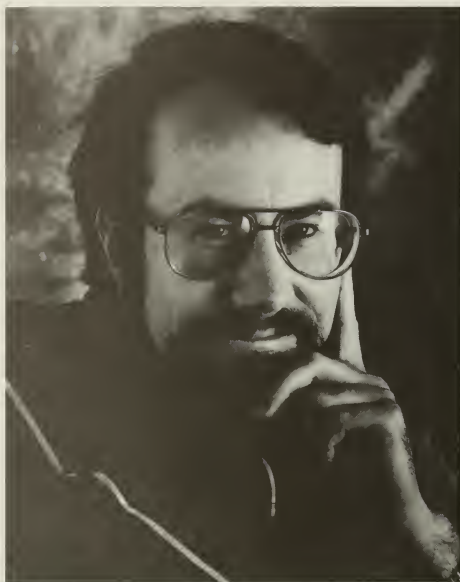
Automobile catalytic converters contain small clusters—on the order of several hundred atoms—of metals such as platinum, palladium, and rhodium. These clusters catalyze the conversion of deadly gases such as carbon monoxide and nitrous oxide to carbon dioxide, nitrogen, and oxygen.

"Rhodium is the element of choice," says Adams, "except for the fact that the whole world's supply of rhodium comes from two mines in South Africa. It's incredibly expensive. We're working to determine the structure of the metal clusters and how the structure affects their catalytic properties. Eventually, we hope to use the results to find less expensive, or more effective, replacements."

Using quantum methods

Experimental data in these projects are scarce, so Adams uses quantum mechanical methods to simulate these systems. While the methods are extremely accurate, they are also slow: he can only include 100 to 200 atoms in his simulations, for very short periods on the CRAY Y-MP system. "There is no way we could do these calculations without NCSA's CRAY Y-MP or their IBM RS/6000 workstations," says Adams. In the

Atomic-level continued on page 18



"It's possible that we could cover substantial areas of the desert with solar cells, for example, and supply most of the electricity for the U.S."

—Jim Adams

Atomic-level continued from page 17

future, Adams' IBM allocations will be transferred to the Cornell Theory Center, which will be the new national metacenter's IBM RISC-cluster hub.

Metallic glasses and interfaces

In yet another potential industrial application, Adams is studying the thermodynamics of metallic glasses. "Metallic glasses are just metals that have random (rather than crystalline) structures—but they have wonderful magnetic properties that make them ideal for use in the core of power transformers," Adams says. They are made by cooling a metal extremely rapidly—"you cool a molten red hot metal to something you can hold in your hands, in about a hundredth of a second," according to Adams. His group is the first to undertake a study of the thermodynamics and stability of metallic glasses. They would like to understand why some elements, and not others, will form glasses under this process.

Lastly, Adams' group studies metallic interfaces—also called grain boundaries. Metals are composed of crystals, all of which may have a slightly different orientation with relation to the other crystals. This difference in orientation results in a defect, which greatly influences the strength or weakness of the metal as well as speed with which impurities can diffuse through the metal. "We've been carrying out the first computer simulation of diffusion in these grain boundaries," says Adams. He points out with matter-of-fact pride that his group is one of the world leaders in understanding surface diffusion on metals.

Adams' work with metallic glasses and metallic interfaces is novel because he combines quantum mechanical first principles calculations with experimental data on bond energies, bond lengths, and the response of atoms to applied forces. "We're the first group to try this method," says Adams, "and it's working surprisingly well. We've found that this method works much better than other empirical models, especially in modeling alloys."

UIUC student benefits

Noting that Adams' work includes a lot of "firsts," he acknowledges that his success is a mixture of having access to NCSA's computational power and his use of novel models for carrying out the simulations.

UIUC students are among the beneficiaries of Adams' work on atomic-level computer simulation. He is teaching a graduate-level engineering course this semester on atomistic computer simulation, in which students use the codes developed on NCSA's RS/6000s to perform their own computer simulations on UIUC's campus-sponsored RS/6000s. ▲

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Ronald Maurice Cosby, Ball State U., "Electron Transport in Nanoconstrictions"

Douglas M. Eardley, Institute for Theoretical Physics, U. of California at Santa Barbara, "Studies of Electronic and Spin Systems"

Adolfo G. Eguiluz, Montana State U., "Dynamical Density Response and Electronic Many-Body Effects in Real Metals"

Jiangdi Fan, Louisiana Southern U., "Computer Simulating Study of High-Temperature Superconductor Structures"

Robert C. Frank, Augustana College, "Trapping of Small Atom Impurities by Lattice Defects in Metals"

Arthur J. Freeman, Northwestern U., "Electronic Structure of Artificial Materials and High-Temperature Superconductors"

Eduardo R. Gagliano, UIUC, "Spin Dynamics in the Cuprate Superconductors"

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Hamlin M. Jennings, Northwestern U., "Computer Simulation of Impedance Spectroscopy of Cement Paste"

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Atom-Surface Collisions

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Allan Hugh MacDonald, Indiana U., "Strongly Correlated Quantum Systems"

Gerhard Müller, U. of Rhode Island, "Dynamics of Spin Systems"

David Pines, UIUC, "Spin Fluctuation Induced Superconductivity"

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Yia-Chung Chang, UIUC, "Electronic and Optical Properties of Growth Surfaces and Doped Quantum Wells"

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Leo P. Kadanoff, U. of Chicago, "Singularity Formation in Surface Tension Driven Flows"

Vadim Kalmeyer, UIUC, "ISTC-Numerical Study of Strongly Correlated Electron System on the Lattice"

Malvin H. Kalos, Cornell U., "Simulation Studies of Quantum Many Body Systems"

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Gabriel Kotliar, Rutgers U., "Quantum Monte Carlo Studies of Strongly Correlated Fermi Systems"

Ronald D. Kriz, Virginia Polytechnic Inst. & State U., "Simulation and Visualization of Stress Wave Propagation near Fiber-Matrix Interphases: Scanning Acoustic Microscope Simulation for Determining Interphase Structure"

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Results of a simulation of a surface layer of helium atoms on graphite. Because of quantum motion, the helium atoms are a probability cloud. The three atoms in the center of the picture are exchanging positions. This results in a ferromagnetic property: they become spin aligned at several thousandths of a degree above absolute zero. The work was done as part of a collaboration between Benard Bernu at the University of Paris and David Ceperley at NCSA. (Courtesy of David Ceperley)

Quantum World continued from page 7

5,000 CPU hours of NCSA's CRAY Y-MP system on NCSA's networked SGI workstations for his research on the effect of disorder on superfluidity.

Clustered workstations are well-suited to QMC methods—many calculations can be conducted relatively independent of each other and then summed.

Exploring new architecture

"People are thinking about how to make their methods more efficient and do a chunk of a complex material like high-temperature superconductors," Ceperley says. "The unit cell, or basic building block, may consist of a hundred atoms or more. Now they can think about putting the whole cell on the computer, whereas before they'd have to take only ten atoms."

Ceperley is exploring the use of new architectures—specifically Thinking Machines' CM-5 system at NCSA—to perform calculations on the electronic structure of condensed matter in collaboration with UIUC Computer Science Professor Roy Campbell and Martin. Their project recently was awarded a grant from

NSF's HPCC Computational Advances in Materials Research (CARM) Initiative [see *access*, October–December, 1992].

The group's goal is to develop methods using massively parallel processing (MPP) computers that can be applied to problems in experimental physics and materials science. They will study properties of materials such as silicon, condensed states of hydrogen, surfaces of metals, and liquid and amorphous systems, superlattices, and correlated electronic states in magnetic insulators.

These studies may lay the foundation for the development of the next generation of computational materials science. Possibly the power of MPP could be used to accurately describe and predict more complex materials and phenomena—such as correlations that lead to magnetism and superconductivity in transition metal compounds.

In another group effort, Ceperley is working with a multicenter collaboration on quantum simulations of molecules and materials. This project involves colleagues from Kent State, Cornell, Arizona State, and New York Universities; University of California at Berkeley; and Brooklyn College.

Ceperley [see *access*, May–June 1992] simulates complex systems with more atoms via the CM-5. This should be particularly useful for materials that exhibit both large- and small-scale quantum behavior. The Path Integral Monte Carlo code is now running on the CM-5 in the MIMD mode. Work on using this code to continue the simulation of hydrogen at high pressure has begun. Recently the Grand Challenge Allocation Committee granted 150,000 node hours on the CM-5 to continue this work.

Technology transfer

New computational methods are developed and then transferred from NCSA to the national materials science community by the Quantum Systems layer of NCSA's Applications Group, which Ceperley heads. In addition to his research, Ceperley provides a voice for materials scientists by defining the capabilities of NCSA's computational environment and determining allocations policy on NCSA architectures. Toward this end, NCSA has hosted a series of international long-term visitors and postdoctoral research associates.

Recent visitors include: Roberto Car [University of Geneva], Detlef Hohl [KFA (German national laboratory), Jülich], Michel Caffarel [Toulouse], and Krauth [Paris]. UIUC postdoctoral associates at NCSA include: Silvia Bacci, Lubos Mitás, and Massimo Bonisegni.

Marcus Wagner, Jeff Grossman, William Magro, and Matt Jones—UIUC graduate research assistants at NCSA—are obtaining first-hand experience with new architectures and methods under Ceperley's guidance. Ceperley is currently participating in an effort within UIUC's College of Engineering to define a new Program in Computational Science and Engineering that will be designed to train students in applying supercomputers to scientific problems.

Ceperley lectures extensively on algorithms at an annual workshop on new methods in QMC. Initiated by NCSA, this practice is now being perpetuated by the condensed matter community. Ceperley plans to give a tutorial on Monte Carlo methods at Physics Computing '93. In the fall of 1993, he will visit the University of Lausanne to further collaboration with Roberto Car on QMC methods.

With Jim Gubernatis (Los Alamos National Laboratory), Ceperley organized a workshop on "Quantum Many-Body Computations for Condensed Matter Physics" to be held in Santa Barbara, CA in spring 1994. It will be attended by colleagues Walter Kohn, Doug Scalapino, and Robert Sugar from Santa Barbara's Institute of Theoretical Physics [see *access*, October–December 1992], as well as other national and international colleagues, including Malvin Kalos (director, Cornell Theory Center) and Car.

Only a start

Materials science is in its infancy. Ceperley points out, "We're still very far from understanding how to solve the equations, but that's only part of the problem. The other part is the possible complexity. After all, even a person is a material. That's how complicated materials can be."

"Biological things are an example of something extremely complex that's just made from a few elements. You can take the elements, and you can mix them in an infinite number of ways. We won't exhaust this science for centuries—probably even millennia." ▲

almost completely line up antiferromagnetically," Pines explains.

He also points out that the location of the spin fluctuations plays an essential role in the high-temperature superconductors. "The magnetic interaction between the quasiparticles is particularly strong at just those regions in momentum space where it can be effective in bringing about superconductivity."

From their calculations, it became clear why the superconducting transition for $\text{YBa}_2\text{Cu}_3\text{O}_7$ occurs at 90K.

The most critical component of the theory concerns the nature of the pairing state. Pines says the theory "makes a major prediction about the nature of the pairing state that describes superconductivity. The relative angular momentum must correspond to d-wave pairing, in which the energy gap for quasiparticle excitations in the superconducting state vanishes along selected directions in momentum space.

"[The] pairing state . . . can be checked experimentally directly to see whether it has any chance of being right," he continues. "If the pairing state is anything other than [that] which our theory predicts, the theory is wrong."

The d-wave pairing differs markedly from the s-wave pairing found in low-temperature superconductors, for which the corresponding energy gap is finite and almost isotropic, Pines says.

During the past few months, the pairing state of the Monthoux/Pines theory has been confirmed by three separate experimental groups. A team led by Walter Hardy, University of British Columbia, has used microwave experiments to investigate the superconducting state, while another team led by Z.-X. Shen, Stanford University, has used angle-resolved photoemissions as a probe.

Newer efforts by Slichter's group at UIUC have again involved NMR, from which Monthoux and Pines first developed much of the spin fluctuation theory. "The results of the NMR experiments were particularly bizarre and unexpected, yet d-wave pairing provides a quantitative explanation."

MPP and new compounds

Despite the crucial role played by NCSA's CRAY Y-MP system in devel-



1972 Physics Noble Prize winners standing in BCS theory order at the ceremony: John Bardeen (late of UIUC), Leon Cooper (now at Brown University), and J. Robert Schrieffer (now at Florida State University). (Courtesy UIUC Dept. of Physics)

oping the spin fluctuation theory, Pines says that the structure of the interaction and the strong coupling effects push the system's limits. "We need more memory . . . to go down to lower temperatures and look at all the properties in the superconducting state."

Monthoux adds that he has exhausted the Fast Fourier Transform (FFT). "We're going to look at a more elaborate model in which the equations are not simple convolutions," he explains. "Then the FFT is of no real use; I will have to use finite elements."

Such work involves very large matrices, which can be efficiently handled on a parallel computer. For these more complex studies, Monthoux will explore using Thinking Machines' CM-5 at NCSA.

While $\text{YBa}_2\text{Cu}_3\text{O}_7$ is the best characterized compound, Monthoux and Pines are beginning to look at other compounds and other families. They recently applied for additional CRAY Y-MP time to study $\text{YBa}_2\text{Cu}_3\text{O}_{6.63}$, a "reduced oxygen" compound.

Applications

Visions for the use of high-temperature superconductors include levitated trains and superconducting supercomputers with much faster connections than those in use today.

Pines says that IBM was working on the latter and that researchers in Japan are working on both applications.

Over time, high-temperature SQUIDS—"if you are clever enough," Pines interjects—could measure tiny magnetic waves from the brain that reflect human thought in a field called *neuromagnetism*. "This is long-term but not science fiction."

Perhaps the ultimate superconductor would lose its electrical resistance at room-temperature (approximately 300K). Then, Pines jokes, people could have them in their homes.

He recalls that in the first flush of enthusiasm following Muller and Bednorz's discovery, researchers were optimistic about reaching much higher temperatures. "It is certainly not impossible," he says, "but you'll have to make a material different from anything being made now."

More realistically, by the year 2000 the threshold for superconductivity could easily be 150K, Pines believes. "Indeed, someone may have already discovered such a material, but they do not have it in a sufficiently stable form." ▲

NOTE: If you are interested in obtaining a videotape about Pines' research into superconductivity, see page 35 of this issue "Back to the videotape."

CITATION

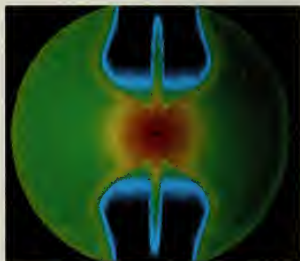
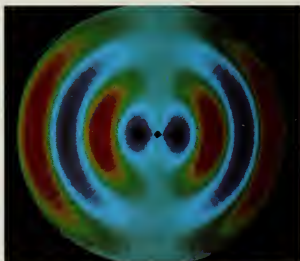
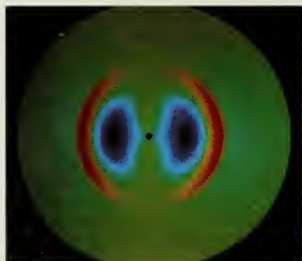
1993 HELEN B. WARNER PRIZE FOR ASTRONOMY

Dr. John F. Hawley

The 1993 Helen B. Warner Prize for Astronomy is awarded to John F. Hawley for advancements in the field of computational astrophysics, and for significant discoveries that have been made with the numerical tools that he developed. A world leader in this emerging discipline, Hawley exhibits a remarkable balance of physical intuition with technical virtuosity and is a creative thinker both in analytical and in numerical science.

Recognizing the great importance of magnetic fields in systems of interest, Hawley invented a powerful new approach to magnetohydrodynamic calculations. Long avoided in the astrophysical community as prohibitively complex, numerical MHD has matured under Hawley's leadership into a powerful computational tool. With this tool, in collaboration with S. Balbus, Hawley discovered the almost universal nature of a powerful MHD instability, which may be the underlying physical cause of turbulent viscosity in accretion disks.

Hawley has also pioneered the application of supercomputers to other aspects of the gasdynamical behavior of accretion disks, in scenarios ranging from fully general relativistic flows onto black holes to the formation of planetary progenitors around ordinary stars.



Accretion of gas onto a black hole—considered the fundamental power source for active galactic nuclei and quasars. (Sequence from "Rotating Gas Accreting onto a Black Hole"; John Hawley and Larry Smarr, principal investigators; NCSA visualization)

John F. Hawley

John F. Hawley has been an assistant professor of astronomy at the University of Virginia since 1987. During 1988 he had a visiting research appointment to the Institute of Theoretical Physics, University of California at Santa Barbara. Hawley has been a member of the joint Peer Review Board for NCSA and the Pittsburgh Supercomputing Center since 1989. He earned his Ph.D. in Astronomy under Larry Smarr at UIUC in 1984 and wrote his dissertation on black hole accretion using numerical analysis. Hawley is one of NCSA's earliest users.

WHAT EDUCATION OUGHT TO BE: PERSPECTIVES OF YOUTH

BY SARA LATTI, SCIENCE WRITER

Fill-in-the-blank worksheets and rote memorization of facts, always an anathema to students, have become even more so to young people accustomed to fast-paced Nintendo games and action-packed television shows. Poor student performance and high student drop-out rates have spurred a national effort in education reform, the topic of an HPCC in Education Seminar, "What Education Ought to Be: Perspectives of the Youth." Lisa Bievenue, NCSA specialist in education, arranged the presentation.

This seminar, held in mid-February at the Beckman Institute, differed from most in one significant respect: the speakers were students—ranging from a third-grader in a Champaign elementary school to a senior in science education at UIUC. Despite their age differences, they were nearly unanimous in their call to harness student creativity in a more hands-on approach to the curriculum.

Hands-on projects preferred
Elaine Schulte, a senior at Centennial High School in Champaign, regards her independent study course in computer-aided chemistry visualization [see *access*, July–September, 1992], which uses one class period and a "considerable amount of out-of-class time," as a treat: "When I finish my English homework, I work on my independent study class because that's what I really enjoy doing," says Schulte. "It makes the education experience more flexible, allowing for some variation depending on the creative ability of the student.



Hands-on projects have helped me more than doing any of the bookwork, such as diagramming sentences, solving problems, or writing papers. It [the bookwork] rapidly becomes very boring, and you don't always understand what's going on."

Emilia Garvey, a third-grader at Champaign's Washington Elementary School, agrees. "The more projects we do, the more about the facts we learn," she says. "In social studies, we are learning about farming communities. Instead of just reading the book and doing the papers, we could talk about how farming communities have changed over the years, and maybe how children in farming communities and children in city communities are different and why. It would be a lot more fun for the children than just listening to someone reading out of a book." Garvey also felt that a wider subject range and allowing for greater

Left to right: James Gasaway, Joseph Smarr, Greg Kolke, Emilia Garvey, and Elaine Schulte.

Perspectives continued on page 24

flexibility in doing schoolwork would stimulate greater interest among elementary students.

Real-life applications wanted

"Most science today comes right out of the textbook," says Greg Kolke, a senior in science education at UIUC. "It's memorization of facts and concepts, with no real understanding. All too often, I see a teacher hand out worksheets and say, 'Here, you work on these while I grade papers.' And that leads to behavioral problems, because the kids don't want to sit there passively doing worksheets." Kolke acknowledges the importance of learning basic terms and concepts, but adds that "true understanding comes when kids work with phenomena out in the real world." Kolke likes to use the phrase "hands-on/minds-on" to describe the kind of learning that takes place when children are allowed to apply their knowledge to real-life phenomena.

Joseph Smarr, a sixth-grader at Urbana Middle School, provided an explanation for why students prefer a more interactive learning environment. When teachers rely heavily on lectures and worksheets to teach the subject matter, "many kids feel that they're not in charge and that they're not making any decisions," says Smarr. Kids spend "endless hours"

on video games, according to Smarr, "because they feel that they can use their brains to make decisions. I think that schools should be aware that kids want to learn with projects because they give them a chance to make a difference. They get to use their own imagination and knowledge." Smarr stresses that, although computers can be a valuable tool in interactive learning, they are not a prerequisite. Acknowledging that many schools have "limited budgets, space, and time," Smarr says that teachers should make use of resources like NCSA. Community centers and libraries could offer computers for interactive learning as well, Smarr said, especially in inner-city areas in which schools have neither the money for computers nor access to a resource such as NCSA.

Last October Smarr made a similar presentation before the National Research Council's Coordinating Council on Education in Washington, DC. He feels that it is important to speak to others about his ideas to encourage change in schools.

High-tech aids for teachers

"We've heard a lot about hands-on activities," says James Gasaway, a junior in science education at UIUC, "but I see a lot of frustration with teachers who say, 'How? What am I going to do? It's easy to hand out a worksheet.'" The key, according to

Gasaway, is teachers helping teachers. "There's always going to be someone who has an idea on what they can do with one specific topic," he says.

There are many electronic bulletin boards for teachers, according to Gasaway, in which individuals can request ideas on incorporating music into science courses, for example, or livening up *Romeo and Juliet*. "It's also possible to create databases on specific areas, which teachers could simply access through anonymous FTP," says Gasaway. "The more teachers get their hands on it, the more it evolves and changes. You don't have to be that creative as an individual anymore; you don't have the burden of coming up with some entirely new idea to get the kids interested."

"One of the barriers to the use of network resources," says NCSA Director Larry Smarr, "is having to spend long distance charges with modems to get to a network. One of the great things about Internet is that a local phone call can get you all over the U.S. for free. We need to make sure that every school in the country has at least one Internet access. I think that this notion of how technology interacts with education is something that Vice President Gore and President Clinton are going to place higher and higher on the national agenda." ▲

Call for more REU interns

Applications are now being accepted for the Research Experiences in Computational Science for Undergraduate Students Program for the next academic year. Deadline for full consideration was April 16, 1993, but applications are still being accepted.

NCSA, with NSF funding, will bring undergraduates from around the U.S. to the center for a semester-long internship of research—either in fall 1993 or spring 1994. Participants will be matched with an NCSA research project in their area of interest. Computational science is the program's focus. Interns, who are selected in a national competition, will receive training in vectorization, parallelization, and visualization.

Junior and senior undergraduate students who are citizens or permanent residents of the U.S. or its possessions may apply. Applicants should be comfortable with the use of computers but need not be majoring in science or engineering.

Applications are encouraged from students at liberal arts colleges, small universities, and institutions serving populations that are underrepresented in scientific/engineering professions.

For application requirements and further information, contact Lisa Bievenue, specialist in education for NCSA's Education Program [see **nca contacts**, page 2].

NCSA's new undergrad internships

*by Jan Alexander, Freelance Writer
photographs by Thompson-McClellan Photography*

* * *

A new program at NCSA open to undergraduate students allows them to discover the role of supercomputing in science and education. The Research Experiences in Computational Science for Undergraduate Students Program, which began in fall 1992, was initiated by Bob Wilhelmson (NCSA research scientist and UIUC atmospheric sciences professor) and Nora Sabelli (NCSA senior research scientist on leave to NSF as program director, Applications of Advanced Technologies). Lisa Bievenue, specialist in Education, and Robert Panoff, senior research scientist in Education, coordinate the program.

Also known as the Undergraduate Internship in Computational Science, the program was created so that students from small colleges and universities could take advantage of the environment at a large research institution for a full semester.

Contributing to NCSA

"We encourage applicants from social science and humanities disciplines as well as basic science departments," says Bievenue. The program, which is open to students in all fields of study, helps students understand how computational science is instrumental in whatever field they choose.

"Because of the time and concentration of effort involved," says Panoff, "it's really an immersion program rather than an internship program." Students generally work 30-40 hours a week on their research projects.

Internships continued on page 26

"They come in as undergrads, but are working at almost a graduate level." Panoff adds, "They contribute significantly to the research environment. For example, many of the results [in the projects] would not have been achieved without their contributions."

Selecting participants

Criteria for student selection includes topic for research, science and computational backgrounds, and overall credentials.

Student interns are matched with mentors who oversee their projects and give training and support. The selection committee seeks a diversity of backgrounds to give participants a range of experiences.

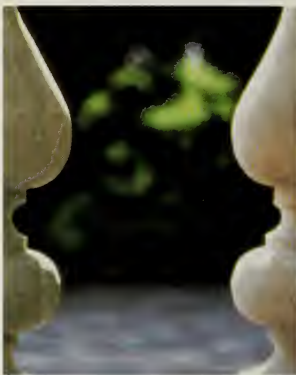
Funding is provided jointly through a grant from NSF and NCSA. Besides a stipend and housing expenses, the program pays for up to five class hours for students who want to take a class at UIUC.

As word gets out about the program, more people apply. Last fall, ten people applied; this spring, 50. Bievenue would like to expand the program and is working on more funding. "The goal this year is to demonstrate the utility of this approach," says Panoff. The hope is that positive results of NCSA's program will encourage other supercomputing centers and universities to offer similar, semester-based programs.

"We're always looking for exciting opportunities for research," says Panoff, who would like to expand the projects available. After this semester ends, he would like to help current students continue researching on their own campuses via Internet. This could enable former students to be electronic mentors for incoming students also.

Broadening experiences

Currently there are five interns at NCSA. Projects this semester include designing mathematics software for elementary students, implementing parallel algorithms, compiling nineteenth-century census data for study, studying light rays in black holes, and predicting the structure and function of proteins.



At weekly seminars, interns get a chance to interact with other REU students from UIUC and exchange ideas [see *access*, September–December 1991]. At one of these seminars, they will also make presentations on their projects.

According to the participants, all feel they have benefitted from the program through access to new resources and ideas. They feel better prepared for graduate school, too.

Developing math software

One of the students enrolled in the program, Michael South from Valdosta State College in Georgia, is studying physics and math. He works with Panoff to develop software to introduce kids to concepts usually only seen in advanced college math, such as abstract algebra and fractal geometry. South sees a need to attract children to math and interest them in it at an early age.

Like others in the program, South had no previous supercomputing experience. Access to the CRAY Y-MP supercomputer has allowed him to do many fractal experiments.

What are the benefits of the program? "There are so many it's hard to put into words. There's so much more I can do here with visualization programs." He says the experience at NCSA has expanded his knowledge of teaching and given him new ways to think about computer applications. South credits Panoff with making the adjustment and training fairly easy.

After leaving NCSA, South plans to pursue a master's degree and would like to teach math at the secondary or elementary level: "There's so many ways to do it [teach] that haven't been explored."

Implementing algorithms for parallelization

Boyana Radenska from Southwest State University, Marshall, MN, is majoring in computer science. Working with Michael Heath, head of NCSA's Mathematics and Computer Science Group, she is implementing parallel algorithms for matrix multiplication and factorization. For this work, she uses parallel computers—the Thinking Machines' CM-5 at NCSA and an Intel iPSC/860 hypercube at Oak Ridge National Laboratory. "He's always there when I have questions," she comments on Heath's helpfulness.

Heath got involved with the program because of his previous involvement in a similar program at Oak Ridge National Laboratory in Tennessee [see *access*, January–April 1992].

Radenska enjoys learning about parallel processing, using the resources available, and meeting new people. She plans to graduate in spring 1995 and go on to graduate school for a Ph.D. in computer science. Afterwards she is considering teaching.

"They [the interns] contribute significantly to the research environment."

—Robert Panoff

Computing and social science

Intern Robert Shaughnessy, from Rockhurst College in Kansas City, MO, is a double major in computer science and political science. Shaughnessy works with Terry Finnegan, NCSA postdoctoral research fellow, to compile nineteenth-century census and other data to show the impact of the Civil War on an area in North Carolina between 1850 and 1890 [see *access*, October–December 1992].

Shaughnessy is working on a code for record linkage, a key function in the project. He likes working on his project because it involves computers and social science. Finnegan says that Shaughnessy has been a helpful addition to the project: "We consider Robert to be our colleague."

Shaughnessy, who takes a UIUC class in artificial intelligence, enjoys the class material. In fall 1993 he plans to graduate and go to graduate school to study computer science, particularly artificial intelligence.

Studying black holes

Joseph Libson, from Washington University, St. Louis, MO, is working with Edward Seidel, NCSA research scientist in gravitation, on a project involving the study of black hole physics. Libson is exploring where light rays go through a system in a black hole.

Seidel and Libson found out about each other, and Libson about the program, through a mutual acquaintance, Wai-Mo Suen of Washington University. Seidel is glad to have Libson's assistance.

Seidel said the program provides good research experience for undergraduates. "Research is not like the textbook learning they're used to," he says. After Libson leaves, Seidel would like to continue having other interns work on his ongoing project. Libson plans to graduate in May 1993 and continue his study of relativity in graduate school.

"We encourage applicants from social science and humanities as well as basic science."

—Lisa Bievenue

Projects in computational biology

Intern Kevin Scott, Lynchburg College of Lynchburg, VA, is working on three research projects in various aspects of protein folding with Shankar Subramaniam, NCSA research scientist in computational biology.

Scott has been busy in his short time at NCSA—completing one project and co-authoring two papers. Collaborating on a coding scheme for storing aligned genetic sequences, he wrote programs to determine nucleic acids like those in the Human Genome Project.

Another project on mutagenesis is in the conceptual stage. Using VIEW, a software program still being tested, Scott will be doing 3D molecular visualizations of proteins to study their structure and sort out their subsets. A third project, again involving visualization, will study aligned sets of structures in proteins. Soon he hopes to move code to the CONVEX C3880.

"Being here," says Scott, "has solidified my goals to go to graduate school and pursue academic research" as a career. His special interest is the knowledge-based approach to machine learning.

While at NCSA, he has "gotten some neat ideas about what kinds of problems biologists studying protein structures need to solve." Scott looks forward to continuing his research via Internet after he returns to Virginia.

A program "graduate" speaks

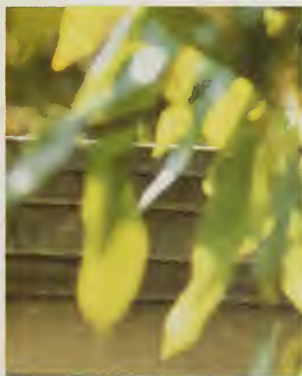
Kara Andosca, who was one of the first interns last semester, recently transferred to the UIUC from the University of New Hampshire, Durham. Her background is in math and physics.

Her NCSA project, also done with Subramaniam, involved the prediction of structure and function of proteins. The information gained in her research could be applied to drug design.

Andosca found the format of the program relatively easy to adjust to because of her enthusiasm for her project, but she advises those interested in the program: "You do have to be very devoted. You have to work really hard." She credits Subramaniam with making the project enjoyable.

She feels the program is good preparation for graduate school because it provides the opportunity to find out what a graduate research group is like. Andosca plans to graduate in spring 1994 and is trying to decide what avenue to take for graduate study—either biomolecular or biophysics research.

Andosca's advice for prospective program participants? "Look at the different projects. If it matches [your interests], do it." ▲



UNITED TECHNOLOGIES IS NCSA'S NEWEST PARTNER

United Technologies Corp. is the newest partner in NCSA's Industrial Program, company and university officials announced March 1.

Based in Hartford, CT, United Technologies provides a broad range of high-technology products and support services to customers in the aerospace, building systems, and automotive industries worldwide. Their best-known products include Pratt & Whitney aircraft engines, Sikorsky helicopters, Hamilton Standard aerospace systems, Carrier heating and air-conditioning systems, Otis elevators and escalators, Norden defense systems, and UT Automotive components and systems. Last year, the company's revenues totaled \$22 billion.

"This agreement is a significant development because it adds one of the world's leading industrial companies to our program," says NCSA Director Larry Smarr. "They have been a pioneer in the use of massively parallel supercomputing for engineering applications in product design and manufacturing. Working with them, we aim to be an example of what the Clinton administration 'Technology for America's Economic Growth' initiative hopes to achieve."

"We're pleased to be joining NCSA," says William T. Thompkins, assistant director of research for Information Systems and Technology at the United Technologies Research Center. "NCSA has extensive experience in high-speed computer networking. They also are well known for effectively applying supercomputing as a tool in solving scientific problems—both of these areas are of great interest to United Technologies."

"United Technologies is a very successful, high-profile global company," says John Stevenson, NCSA's corporate officer. "It has a strong position in several key markets as a result of its commitment to be at the leading edge of new technology. We will all benefit from the partnership."

The initial 12-month agreement, including a two-year option, adds United Technologies to a group of ten other NCSA partners: AT&T, Caterpillar, Dow Chemical Co., Eastman Kodak Co., Eli Lilly & Co., FMC, J.P. Morgan, Motorola Inc., Phillips Petroleum Co., and Schlumberger. ▲

"A GLOBAL SOLUTION"

This first joint video production of the metacenter presents the benefits of computational science and engineering to American business. Combining live action footage, visualizations, digital effects, and original music, the video is targeted at Fortune 1000 upper management. It will be used in outreach to industry by the four NSF high-performance computing centers.

Project leader David Curtis produced and directed the video in consultation with the other three NSF-sponsored centers. Robert Patterson, Tony Baylis, Jay Rosenstein, and Robin Bargar of NCSA's Scientific Communications and Media Systems Group made major creative and technical contributions. Additional production support was provided by San Diego Supercomputer Center's VisLab. The project was funded by NSF.

Caterpillar wins 2nd annual NCSA Industrial Grand Challenge Award...

Read all about it in the next issue of access.

SPECIAL INTEREST GROUP IN CFD BY JOHN LURANC, FMC CORPORATION

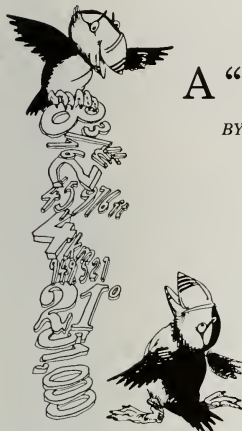
The formation of the NCSA Industrial Partners' Special Interest Group in Computational Fluid Dynamics (SIGCFD) was announced at a meeting held in Chicago attended by Caterpillar Inc., The Dow Chemical Co., FMC Corp., Schlumberger Inc., and NCSA.

The objective of this SIGCFD is to create new tools and capabilities for the application of CFD technology by enhancing the effectiveness of technology collaboration between academia, industry, and the national high-performance computing centers.

SIGCFD's focus is on areas of interest to industry related to research in theoretical and experimental fluid mechanics, and the establishment and validation of new and existing numerical models for simulation. Initially the emphasis will be on internal flows in systems and equipment. Included will be the development of parallel algorithms, to enable CFD problems to be solved efficiently by employing emerging SIMD and MIMD architectures. ▲

A "WHOLE DATA CATALOG" FOR RESEARCHERS

BY FRAN BOND, PUBLICATIONS EDITOR ♦ ILLUSTRATIONS BY ERIC PERUVKHIN



Column data.

Brand Fortner's book, *The Data Handbook: A Guide to Understanding the Organization and Visualization of Technical Data*, is just what its subtitle states. One might call it the "whole data catalog" for organizing, analyzing, and visualizing large datasets gathered from computational research.

Definitely friendly to Macintosh and UNIX users, a "Quick Tour" of how to get the most from the book is a useful part of its introduction. As one would expect, organization is paramount in this text. Readers are even guided to various levels of coverage: "For Real Techies," "For Serious Techies," and "For Ultra Techies."

Aside from the point that almost everything a computational researcher would want to know about handling and visualizing data—from 1D to 6D—is included, some interesting facts are learned from the book as well. For example, one finds that "An ASCII text datafile can take two to five times the disk space of a comparable binary datafile." And: "2D matrix datasets take up much less disk space than column datasets for data on a regular two-dimensional grid."

Thoroughness is a hallmark of this guidebook. For instance, line and bar graphs (1D), scatter and parametric plots (2D/3D), and scatter matrix plots (6D) are all considered in Chapter 7, "Column Data." Definitions of computer terminology are excellent as well.

Scattered throughout the text are examples that use data from five fictitious researchers—Judy ReSyrch, Michael Astroe, Dr. Tim Boans, Jeanne Beeker, and Wolfram Herth. They not only reinforce the book's concepts, but keep it from being dry.

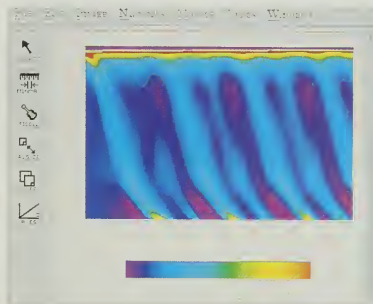
This is one of the most engaging technical texts on the market today. Eric Peruvkhin's drawings of puffins (left and below) delightfully and appropriately introduce each chapter.

About the author

Fortner is a founder and director of research and development for Spyness Inc., an NCSA spin-off company founded in 1990. Producing accessible data visualization software for UNIX operating systems and Macintosh computers is its specialty (above right). The book may be obtained from Spyness Inc., P. O. Box 6388, Champaign, IL 61826.



Floating point numbers.



Spyness Transform 3.0 for UNIX and Macintosh. (Courtesy of Spyness Inc.)

Next month *The Whole Internet* by Ed Krol will be reviewed. Krol worked at NCSA in its early days as network manager and oversaw the installation of NSFNET for UIUC.

New book

Supercomputing and the Transformation of Science, by William J. Kaufmann III and Larry L. Smarr, was recently published by Scientific American Library (distributed by W. H. Freeman and Company, New York and London). The book has been reviewed in a number of publications, including *Nature* and *Science News*. Dedicated to "intellectual giants who made the digital world possible," it ranges from the historical development of supercomputing to over 100 exemplary descriptions of research in the computational sciences. It contains some 200 color images. ▲



NCSA Director Larry Smarr (center) shakes hands with Larry Shelby (left), Urbana businessman and member of the board of directors for the Champaign County Chamber of Commerce, as Smarr moves towards the head table with his wife Janet, director of UIUC's Comparative Literature Program. Speaking on "Where Will the Development of the Silicon Prairie Be in 2000?" at the group's annual dinner, Smarr said there are "all kinds of new ways for people to be thinking about how to do things" via state-of-the-art telecommunications and computing technology. Citing examples of how this technology is already benefitting other communities, he challenged the group to lead the way in the local area. Smarr offered to work with a task force of local leaders to develop plans that could add value to the local community by utilizing advanced technology. Through the computational resources of NCSA and UIUC, Smarr said that "something grand" could be accomplished in the community by the year 2000.

CRAY-2 TO BE REMOVED FROM SERVICE IN MID-AUGUST

BY SCOTT LATHROP, ASSOCIATE
DIRECTOR FOR USER SERVICES

NCSA's high-performance systems continue to evolve in response to technological developments and requirements of the scientific and engineering communities. The supercomputers and advanced tools available at NCSA have been the focus for our research, development, and educational thrusts with our users.

At this stage in our evolution, we are taking stock of the technological growth and innovations in computing. Because of changes, NCSA has decided to retire the CRAY-2 system from service in order to invest our limited resources (money and staff time) in bringing massively parallel processing into the mainstream of computational science and engineering. This action will accelerate the potential for accomplishing breakthrough science.

As the national meta-center grows in terms of available computing power for researchers, each machine must be assessed in terms of the cost of providing access (maintenance, environmental, etc.) versus the computing capacity available to the national community.

Initially the CRAY-2 system was installed to

service applications with both high computational and large memory needs. In the past year, NCSA added both a massively parallel Thinking Machines' CM-5 and a large-memory CONVEX C3880 to the national metacenter. At the same time, Pittsburgh Supercomputing Center (PSC) added a CRAY C-90 vector multiprocessor.

The table below shows the relative computing and memory capacities (in terms of total memory size and total computational throughput) of these machines. The computing capacity of the CRAY-2 system at NCSA has been replaced many times over by newer machines available at NCSA and at the other NSF centers.

NCSA plans to remove the CRAY-2 system from national service at mid-August, 1993. All current allocations on the CRAY-2 system will be moved to the CRAY Y-MP system by August 1 to allow researchers to continue their work. The Peer Review Board, which acts jointly between NCSA and PSC, is now allocating some of NCSA's requests for Cray time on PSC's CRAY C-90 system.

Through October 1, 1993, the PRB will continue to allocate time on the CRAY

Resource	Location	Total memory	Peak throughput
CRAY-2	NCSA	1 GBYTE	2 GFLOPS
CONVEX C3880	NCSA	4 GBYTE	2 GFLOPS (32 bit FP)
CRAY C-90	PSC	4 GBYTE	16 GFLOPS
TMC CM-5	NCSA	16 GBYTE	64 GFLOPS

Y-MP system at NCSA. The CRAY Y-MP system will remain in service until October 1994, when its lease is over.

During the coming year, NCSA will be working with our academic and industrial constituencies, our funding agencies, and the vendors to evaluate our direction for technological growth and future machine acquisitions.

If you have any questions about these changes, please contact NCSA Consulting or Scott Lathrop [see **nscs contacts**, page 2]. ▲

APPLY FOR METACENTER MPP INSTITUTE

NCSA and SDSC are collaborating to hold simultaneous MetaCenter Computational Science Institutes on Parallel Computing August 9–20, 1993.

Undergraduate and graduate students, faculty, and industrial partners are encouraged to apply by June 25, 1993. Registration will be limited at both sites.

You should have already received a flier, which included an application.

If you have any questions, contact NCSA's Alan Craig [see **nscs contacts**, page 2] or SDSC's Tricia Koszycki at San Diego Supercomputer Center, P.O. Box 85608, San Diego, CA 92186-9784 [phone (619) 534-5000].

NOTE: The institutes are subject to NSF approval and funding. ▲

ATTENTION ALL NCSA USERS! FILES MIGRATING FROM CFS TO UniTree

BY ARLAN FINESTEAD, RESEARCH PROGRAMMER,
COMPUTING AND COMMUNICATIONS

UniTree, NCSA's new archival storage system, entered production in May 1993 [see *access*, October–December 1992]. UniTree is replacing the Common File System (CFS) archival storage system.

For more details about the migration, see the following *data link* articles: "Mass storage migration begins spring 1993," November–December 1992; "Prepare now for the migration from CFS to UniTree," January–February 1993.

If you currently have access to the CFS archival storage system, you were given access to the UniTree archives. The Internet address of the UniTree archival system is mss.ncsa.uiuc.edu (141.142.3.2).

Tentative migration schedule: 1993*

April–May	Users removed unneeded files from CFS
May	UniTree entered production; NCSA computer users had access to UniTree and CFS
June 4	CFS went into READ-ONLY mode
June 9	CFS files could be accessed via /CFS directory in UniTree
June 30	CFS is turned off
Sept. 30	Files remaining in CFS are permanently removed from NCSA's archival system

* All dates are subject to change. Watch for banner messages for exact dates.

NOTE: If you will be gone from May to Sept. 30, please contact NCSA Operations at help@ncsa.uiuc.edu or (217) 244-0710.

The amount of data you can store in the UniTree system will be restricted based on a quota system. Each user will be given a soft quota and a hard quota. The soft quota will determine how much data you can store in the UniTree system over an extended period of time. You will be able to exceed your soft quota limit, however, and store additional data—up to your hard quota limit—for a period of seven days. When the seven-day grace period expires, you will not be able to store any additional data until you bring down your storage usage under the soft quota limit. To determine your current storage usage and your quota limits, you will use a quota command in FTP.

In early May you were notified by electronic mail about how much data you have stored in CFS and what your UniTree quota limits are.

Watch for other articles, email, or banner messages with detailed information about the mass storage migration to UniTree. In particular, look for an online news article about how to use UniTree.

The NCSA UniTree user's guide is available online via anonymous FTP, Gopher, and ncsainfo. The user's guide is also on UniTree in the /DOCUMENTS directory; you can retrieve it by FTPping to UniTree (mss.ncsa.uiuc.edu). A free copy of the NCSA UniTree User's Guide is available from orders@ncsa.uiuc.edu

If you have any questions, contact the NCSA Consulting Office [see **nscs contacts**]. ▲

1993 SUPERQUEST WINNERS

Schools that will be attending the SuperQuest Summer Institute at NCSA July 12–30 are as follows:

Bob Jones High School, Madison, AL

Gina Sullivan and Teresa Tarter, teacher-coaches
"Plasma Sheath Effects on Ion Collection by a Pin-hole," Keri Kolumbus, Robert Wessly, Timothy Yen, and Dan Zugrav

Illinois Mathematics and Science Academy, Aurora, IL

David Workman and Mark Horrell, teacher-coaches
"Collective Behavior in Gnats," Kurt Gimmel, Ashley Morgan, Ryan Pierce, and Russel Simmons

Riverside University High School, Milwaukee, WI

Blaine Wisniewski and Cullen Carey, teacher-coaches
"Determination of Functional and Evolutionary Relationships in DNA Sequences by Auralization," Jemiah Aitch, Charles Collins, Jeffrey Prichard, and Lorna Schilleman

Montgomery Blair High School, Silver Spring, MD

Susan Ragan and Robert Yee, teacher-coaches
"Analysis and Modeling of Congressional Roll Call Votes," Brooke Dombek
"An Extension of the Controlled Random Search Procedure for Function Optimization," Daniel Chen
"Applications of 2D Cable Theory in the Analysis of Electrocardiac Impulses," Manish Tripathi
"Supercomputer Analysis of Holographic Interferograms for Displacement Using the Fourier Transform Method," Daniel L. Gould ▲



1993 NCSA WORKSHOPS

May 19-21
Computing in the Social
Sciences 1993 Conference

May 24-28
Advanced CM-5 Workshop

July 12-30
SuperQuest Summer
Institute 1993

July 26-30
High School Chemistry
Visualization Workshop

August 9-20
MetaCenter Computational
Science Institute on
Parallel Computing

Academic users, contact
Deanna Walker at
dwalker@ncsa.uiuc.edu or
(217) 244-4198. Industrial
partner users, contact
your representative.
For information about
education workshops,
contact Lisa Bievenue at
bievenue@ncsa.uiuc.edu
or (217) 244-1993.

NOTE: Dates are subject to
change. A cost-recovery fee
may apply to some sessions.
You must register for work-
shops at least 10 days before
the session. ▲

NCSA MOSAIC SOFTWARE

NCSA Mosaic—a global
hypermedia-based informa-
tion discovery, retrieval,
and collaboration system—
has been released by
NCSA's Software Develop-
ment Group.

This new application is
part of NCSA's effort to
develop an environment
to facilitate wide-area,
network-based information
analysis and collaboration
on the desktop.

The X Window System
version is now available.
Those interested in obtain-
ing NCSA Mosaic for the
X Window System can
access it through NCSA's
anonymous FTP server.
Project files are in direc-
tory /Mosaic (For down-
loading instructions, see
the inside back cover.)

Mosaic builds on top of
existing systems, network
protocols, and information
resources currently avail-
able on the Internet, such
as FTP, Usenet news,
Gopher, WAIS, CERN's
World Wide Web, and
NCSA's Data Management
Facility.

See the next issue of
access for more details
about NCSA Mosaic. ▲

SUPERCOMPUTING '93: CALL FOR PARTICIPATION

What: The Conference on
High Performance Comput-
ing and Communications
(HPCC)

Where: Portland, OR

When: Nov. 15-19, 1993

How: Sponsored by ACM
SIGARCH and the IEEE
Computer Society

You can become a part of
Supercomputing '93, the
fastest growing conference
in HPCC, by submitting a
paper or a proposal for a
panel, workshop, tutorial,
research exhibit, or poster.
Submission contacts follow.

**Papers, panels,
posters, and research
exhibits:** Dona Crawford,
Program Chair, Supercom-
puting '93, Sandia National
Laboratory, D1900,
Livermore, CA 94551-0969;
(510) 294-2628 (phone);
(510) 294-3422 (fax);
dona@sandia.llnl.gov

**Tutorials and work-
shops:** Joanne Martin,
Tutorials and Workshops
Chair, Supercomputing '93,
IBM Corporation, MS 601,
Neighborhood Rd., Bldg.
201, Kingston, NY 12401;
(914) 385-9572;
jlmart@kgvnmv.vnet.ibm.com

Proposal deadlines:

**Papers, panels,
tutorials, and work-
shops:** April 1, 1993

**Heterogeneous
Computing Challenge
(part of the research
exhibits):** June 1, 1993

**Posters, video posters,
and research exhibits:**
August 2, 1993

Other contacts:

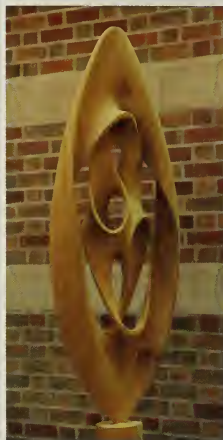
Exhibit space: Don
Collier, DC Expositions,
Inc., (214) 727-8301;
collier@convex.com.

Student volunteers:
Michael Cox, Supercomput-
ing '93 Student Volunteer

Chair, Northwest Regional
SuperQuest Center,
(503) 642-2727;
mc Cox@cse.ogi.edu

For additional informa-
tion, request a "Super-
computing '93 Call for
Participation" by calling
1-800-GO-2-SC93 [1-800-
462-7293] (phone and fax).

Current conference
information is available
through anonymous ftp
at SC93-info.llnl.gov ▲



**Wood sculptures by Brent
Collins.** Exhibit sponsored
by NCSA in the atrium of the
Beckman Institute. Collins' work, executed mostly in
wood, is reminiscent of the
mature work of some early
modern masters like
Constantin Brancusi (1876-
1956) and Antoine Pevsner
(1886-1962). Although not a
mathematician, Collins links
art with topology in his forms.
All the works are untitled.

StarTech A.K.A. CM-5 TIES FOR THIRD PLACE

"Bradley reports a draw in round two (and that the CM-5 performed well all day.)"
Curt [Canada, NCSA]

"... StarTech (playing white on the 512 node CM-5) drew by repetition against Hitech (StarTech's evil twin).

"In this game, StarTech came out of the opening book in a rotten position, was outplayed in the midgame, and outsearched from the midgame on. However, we scrambled back to a moral victory by finding a draw by repetition (through perpetual check) through a rook sacrifice.

"StarTech has now played the number 3 and 4 seeded programs, winning one and drawing one."

Bradley [C. Kuszmaul, MIT]

"StarTech, playing white on the 512 Node NCSA CM-5, drew round 5 against Cray Blitz, playing black on a 16 Processor C-90 located at Cray Research's production lab. (It is a 3-way or 4-way tie for third, depending on the result of one unfinished game.)"
Curt [Canada, NCSA]

Such online interchanges reflect the excitement generated over the 1993 International Computer Chess Championship. This year, NCSA played a part in the annual event sponsored by the Association of Computing Machinery (ACM). A program called StarTech, running on NCSA's CM-5, was the actor.

StarTech tied for third place in round 5. According to Richard Title, Thinking Machines Corporation, "StarTech seems to play a better endgame than most computers... it used its endgame skills to squeeze out wins from small advantage."

StarTech's team members were Bradley C. Kuszmaul, Charles Leiserson, Ryan Rifkin, and James Schuyler at MIT. Working with others, they ran a highly parallel alpha-beta algorithm on NCSA's 512-processor CM-5. Using the Hitech static evaluation function written by Hans Berliner, Carnegie Mellon University, the MIT team reported running at 200,000 nodes/second.

"Because of NCSA's support," says Leiserson, "we were able to substantiate that this load balancing strategy can be used in a production environment to control dynamically growing, real-time MIMD computations.

"The other entrants in the chess competition were quite impressed with the strength of our program on its first outing. Despite the fact that we had no real chess knowledge in our search procedure... the brute force of the CM-5 allowed us to outsearch many of our competitors. We achieved an average speedup of over 100 on the 512 processors of the machine, searching in some cases up to 400,000 positions per second.

We now intend to apply our engineering experience with dynamic MIMD computations to more practical problems. If NCSA has any users interested in branch-and-bound optimization or other problems for which our software technology might be applicable, I would be happy to discuss with them how we might effectively share it."

NCSA research programmers Curt Canada and Michael Welge coordinated the effort.

For further information, contact Charles Leiserson at cel@theory.lcs.mit.edu



LECTURES HONOR ALPERT AND HANNON

"*But Is It True?* Toward a Citizen Understanding of Science and Technology" was the title of Aaron Wildavsky's Sixth Daniel Alpert Lecture in mid-March. Wildavsky, public policy analyst from the Survey Research Center at the University of California at Berkeley, spoke to honor **Dan Alpert's** "continuing interest in promoting communication across disciplinary boundaries." Founding director of the UIUC Center for Advanced Study and former dean of Liberal Arts and Sciences, Alpert is a special consultant to NCSA's Applications Group.

Bruce Hannon, NCSA research scientist and UIUC professor of geography, was honored with the designation of Jubilee Professor of Liberal Arts and Sciences on the College of Liberal Arts and Sciences' seventy-fifth anniversary. "In Loco Naturae" was the subject of the lecture given at mid-April to recognize Hannon's "outstanding scholarship and teaching."



CALL FOR PAPERS IN CHEMISTRY

Presentations are requested for "Theoretical and Computational Approaches to Interface Phenomena," a conference of interest to computational chemists. The conference will be held in Brookings, SD—site of the South Dakota State University—August 2-4 of this year. Proposals for presentations are wanted as soon as possible.

For more information, contact: Harrell Sellers, Department of Chemistry, South Dakota State University, Brookings, SD 57007; (605) 688-6374; hsellers@ncsa.uiuc.edu or Joseph Golab, Amoco Chemical Company, P.O. Box 3011 C-6, Naperville, IL 60566; (708) 961-7878; jtgolab@nap.amoco.com



NCSA STAFF AND REL STUDENTS PRODUCE CNN OPENER

BY JARRETT COHEN, STAFF ASSOCIATE, DIRECTOR'S OFFICE



Still of DNA molecule sequence from CNN's *Science and Technology Week* opener. (Courtesy Robert Patterson and Donna Cox, NCSA Scientific Communications and Media Systems Group)

Every weekend U.S. TV viewers will be seeing the computer graphics of NCSA staff and Renaissance Experimental Laboratory (REL) students in the new opening sequence for Cable News Network's (CNN) *Science and Technology Week*.

The 15-second opener, which began in January, incorporates elements of virtual reality, biochemistry, high-definition technologies, and earth sciences.

Appearing first is a representation of fiber optics, which symbolically connects viewers to the world of science and technology. A dataglove then points to a virtual space inside a notebook computer, where we meet a DNA molecule, a swimming jellyfish, a buckyball, and a human head symbolized by water droplets. The head turns to look at a high-definition computer screen, where we see a detailed, satellite-like view of earth. An astronaut greets us and flies into outer space, with stars forming the title of the show.

The animated elements were rendered separately and then composited for the opener to allow flexibility in refinements. CNN uses the separate elements as story transitions and to announce the availability of teaching materials.

Donna Cox (codirector), Robert Patterson (research programmer), and Michael McNeill (research programmer) of NCSA's Scientific Communications and Media Systems Group developed the concept and produced the animation.

REL students Steve McCure, Michael Moore, and Chris Waegner developed most of the computer graphics models for the production. NCSA Research Scientist Shankar Subramaniam consulted with students on the accuracy of the scientific models.

CNN personnel involved include Bailey Barash, *Science and Technology Week* executive producer, and Ann Williams, vice president for graphics. Atlanta composer Herb Avery wrote the original, image-enhancing score, which was recorded by a small orchestra.

Science and Technology Week appears on CNN on Saturdays at 11:00 a.m. and on Sundays at 12:30 p.m. (Eastern time). This opener will air for two years.

The REL was the subject of a CNN story in November 1992. ▲

COMPUTING FOR THE SOCIAL SCIENCES CONFERENCE MAY 19-21, 1993

NCSA hosted the Computing for the Social Sciences (CSS93) conference at UIUC, May 19-21, 1993 [see *access*, October–December 1992].

NCSA recognizes the need of the social science community to expand the scope and scale of social science research through the use of high-performance computing environments. High-performance computing can provide social scientists with the resources necessary to effectively address large-scale Grand Challenge problems.

With a theme of "Grand Challenges for the Social Sciences," CSS93 helped attendees understand what constitutes a "Grand Challenge" in the social sciences. CSS93 participants were introduced to the uses of high-performance computing for data collection and analysis, theory development and testing, global and social modeling, and social science visualization.

Participants had the opportunity to review thirteen selected CSS93 probe projects—spanning a variety of disciplines and employing high-performance computing in innovative ways to solve previously intractable problems. Participants also attended tutorials and seminars featuring the latest developments in high-performance and microcomputing technology and its uses in research and in the classroom. Several speakers of national renown addressed the conference. (See the next issue of *access* for details.)

Vendors and independent researchers demonstrated software and hardware of interest to the social science community. An additional workshop on interactive access to the 1990 U.S. census was offered Saturday, May 22.

NCSA gratefully acknowledges financial support for CSS93 from the following sponsors: Apple Computer Corporation, College of Liberal Arts & Sciences at UIUC, CONVEX Computer Corporation, IBM Corporation, NSF, SAS Institute Inc., SPSS Inc., and Thinking Machines Corporation. ▲

AVAILABLE NOW: AFS

NCSA recently began using the Andrew File System (AFS), a distributed file system with a common name space. Data are stored in volumes on AFS file server machines and accessed through a cache manager on AFS client machines.

If you work at different sites that have AFS cells (for example, NCSA and the Pittsburgh Supercomputing Center), you and other members of your group can access your data without doing file transfers.

The *NCSA AFS User Guide* is available on NCSA's anonymous FTP and gopher servers and through the online information system *ncsainfo* (on the HPCC systems). A hardcopy of this guide may be obtained free of charge by sending electronic mail to orders@ncsa.uiuc.edu.

For help with using AFS, contact the NCSA Consulting Office [see *ncsa contacts*, page 2]. ▲

BACK TO THE VIDEOTAPE

BY DAVID CURTIS, CODIRECTOR, SCIENTIFIC COMMUNICATIONS AND MEDIA SYSTEMS

In the latest edition of our video magazine, *NCSA RealTime* #6, four new stories portray people, tools, and applications that are at the forefront of HPCC.

Ripples from the Chasm: Probing the wrinkles of space-time. Einstein's theory of relativity, one of the pillars of modern physics, embodies equations that have never been solved in their full generality. A simplified solution has been found: it defines the behavior of one of the most exotic objects in space—the black hole. Led by NCSA Director Larry Smarr and NCSA research scientist Ed Seidel, NCSA's Gravitation Group uses advanced computational techniques and hardware to simulate this ultimate gravitational abyss. The results could light the way towards a numerical solution of Einstein's theory.

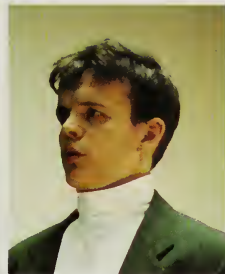
Showcase. A glimpse of science in the next century. SIGGRAPH is the premier annual expo for the international computer graphics community. Among several hundred exhibits at SIGGRAPH '92 in Chicago, one of the biggest crowd catchers was Showcase. Demonstrating the power of real-time, interactive computing and visualization across high-speed national networks, the exhibit presented more than a dozen leading-edge applications from molecular dynamics to cosmology. This piece documents the contributions to Showcase of the NSF-supported high-performance computing centers. Also featured is the CAVE, a highly immersive virtual reality environment created by UIC's Electronic Visualization Laboratory.

Path of Least Resistance. Sleuthing superconductivity's secrets. Superconductors, exotic materials that conduct electricity with no resistance, may eventually change electronics as we know it today. In the meantime, scientists continue the struggle to understand the physics of superconductivity. It's a challenge that has occupied UIUC physicist David Pines for 40 years, beginning with his collaboration with legendary physicist and two-time Nobel Prize winner John Bardeen. Tapping into NCSA's resources, Pines is developing unique insights into high-temperature superconductivity.

Renaissance Renewed. A classroom at the crossroads. Since its founding in 1989 by computer artist Donna Cox (NCSA codirector of Scientific Communications and Media Systems), NCSA's Renaissance Experimental Laboratory (REL) has served as a meeting ground for scientists, artists, mathematicians, musicians, graphic designers, and computer engineers. Equipped with state-of-the-art software and hardware networked to NCSA's most powerful computers, the REL continues to serve as a crucible for the development of new paradigms of visual communication and a conduit for knowledge transfer. Aside from producing world-class imagery, this unique interdisciplinary classroom links training in visual representation and communication to real-world applications in science and engineering, broadcast television, pub-

lishing, and the fine and applied arts.

If you wish to order this edition or previous editions of *NCSA RealTime*, contact Orders for Publications, NCSA Software, and Multimedia [see *ncsa contacts*, page 2]. ▲



Kimmo Koski, manager of Systems Support at Finland's Centre for Scientific Computing, recently spoke on meta-computing in Finland to an NCSA audience. His visit was sponsored by Charles Catlett, associate director for NCSA's Computing and Communications Group, who was in Finland last fall.

(Photo by Fran Bond)

"[NCHPC] will raise the country's perception of what it can do," says NCSA Director Larry Smarr. "The country can achieve more than it is doing."

Smarr continues, "We've got to find a way for the country to advance quickly." He says no one research center can do it alone; "interconnectedness" is the answer. He believes the National Consortium for High Performance Computing (NCHPC) has the potential to be the key—especially with the Clinton administration's focus on supporting new technologies for economic growth.

NCHPC's scope

The goal of NCHPC is to advance massive parallel processing (MPP) systems and technology so that scalable computing is available nationwide. Smarr says that this national effort will cut across agencies and centers in a "macroeffort" capturing the centers' "microeffect."

By developing and extending MPP with the consortium's extensive resources, Smarr says the ultimate goal is to create "one national computational environment." Currently a "set of machines in each vendor class" is being collected toward this end. According to Smarr, "virtually every vendor is involved." Some experimental architecture is being explored at MIT's Laboratory for Computer Science also.

A national distributed, scalable computing environment and a "poststate-of-the-art network system" will make the powerful national machine room a reality. Development and implementation of NCSA Mosaic software (see page 32) is one of the first steps

in this direction. Smarr says that eventually most of the five gigabit testbeds will be meshed together for NCHPC.

Schools K-12 will join in over an expanded Internet, and communities will be networked in as well. Interdisciplinary research partnerships of members from industry, government, and academe are anticipated.

NCHPC's development

NCHPC was formed by Advanced Research Projects Agency (ARPA)* and NSF in response to a call made by ARPA in July 1991 for a collaborative organization focused on scalable high-performance computing. In response, the rest of calendar year 1991 was spent writing and submitting proposals for NCHPC's formation. One of NCSA's earliest moves was to form the Teracomputing Consortium with the Pittsburgh Supercomputing Center and the Naval Research Lab.

Five consortia were chosen by ARPA to comprise the NCHPC (see sidebar), which is a consortium of consortia. In an announcement at Supercomputing '92, ARPA officially confirmed the consortium.

*formerly DARPA

All except one of the original consortia requested funding to buy MPP hardware. Three purchases were made in 1992, including NCSA's CM-5 [see *access*, May-June 1992], which went into production in May of this year.

Research teams

"Right now it is more important," Smarr says, "to focus on the application teams that are developing" through the consortium to see "what comes out."

Six major research program areas have been designated. They are geophysics and astrophysics, chemical and biological sciences, solid state and elementary particle physics, computational fluid dynamics/structures, computational algorithms, and architectures and software tools.

Each research area contains several subprograms. To date, 25 have been defined. Their findings will be shared through workshops.

NCSA's Mathematics and Computer Science Group, led by Michael Heath (NCSA research scientist and UIUC professor of computer science), is the center's liaison to the NCHPC. ▲

CONSORTIUM MEMBERS

Front Range Consortium

National Center for Atmospheric Research (NCAR)
Forecast Systems Laboratory,
National Oceanic and Atmospheric Administration (NOAA)

Center for Applied Parallel Processing, University of Colorado

Defense Supercomputing Research Alliance

Sandia National Laboratory
Army Research Laboratory
Phillips Laboratory

SCOUT: User-builder Synergy for High Performance Computing and Communications

Laboratory for Computer Science, MIT
MIT
Harvard University
Boston University

SuperPar: The Parallel Supercomputing Consortium

San Diego Supercomputer Center
Naval Command Control and Ocean Surveillance Center

Teracomputing Consortium

Naval Research Laboratory
NCSA
Pittsburgh Supercomputing Center

U.S. Chamber of Commerce

Chamber and Community Learning and Information Network

data link discontinued

March-April 1993—volume 7, number 2—is the final issue of NCSA *data link*. Online and printed versions of NCSA's technical newsletter will no longer be available after that edition.

Information regarding user policies, system changes, and NCSA-produced software and tools will appear in a new department of *access*. Documentation for new hardware and NCSA-produced software will continue to be online. Announcements requiring a timely response will be posted online as well.

abbreviations

ARPA	Advanced Research Project Agency
CRI	Cray Research Inc.
CSRD	Center for Supercomputing Research and Development
HPCC	High Performance Computing and Communications
MPP	Massively Parallel Processing
NASA	National Aeronautics and Space Administration
NCAR	National Center for Atmospheric Research
NCSA	National Center for Supercomputing Applications
NRAO	National Radio Astronomy Observatory
NSF	National Science Foundation
TMC	Thinking Machines Corp.
UIC	University of Illinois at Chicago
UIUC	University of Illinois at Urbana-Champaign

downloading from anonymous FTP server

A number of NCSA publications are installed on the NCSA anonymous FTP server. If you are connected to Internet, you can download NCSA publications by following the procedures below. If you have any questions regarding the connection or procedure, consult your local system administrator or network expert.

1. Log on to a host at your site that is connected to Internet and is running software supporting the FTP command.
2. Invoke FTP by entering the Internet address of the server: `ftp ftp.ncsa.uiuc.edu` or `ftp 141.142.20.50`
3. Log on using anonymous for the name.
4. Enter your local login name and address (e.g., `smith@ncsa.uiuc.edu`) for the password.
5. Enter `get README.FIRST` to transfer the instructions file (ASCII) to your local host.
6. Enter `quit` to exit FTP and return to your local host.
7. The NCSA publications are located in the `ncsapubs` directory.



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National Center for Supercomputing Applications
152 Computing Applications Building
605 East Springfield Avenue
Champaign, IL 61820-5516

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Fall 1993 vol. 7 no. 2 High-performance computing magazine

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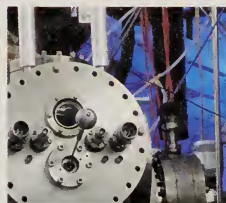
departments

- 2 ncsa contacts
- 3 editor's note
- 34 book review
- 35 center activities

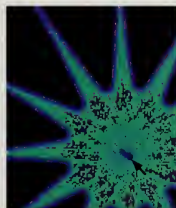


Cover: A collection of antique engineering and surveying instruments. Loaned by the UIUC Department of Mechanical and Industrial Engineering, Berns Clancey & Associates PC, and Fran Bond. (Art director, Carlton Bruett; research, Fran Bond; photography, Thompson-McClellan Photography)

ers
project
eport
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education

27 ISDN links C-U schools to NCSA

28 Software for math & science

29 1993-94 REU members

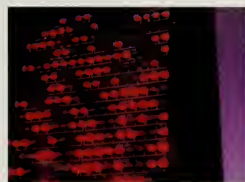
new technology

30 HP, Convex team with NCSA . . . for scalable applications research

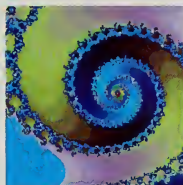
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Fall 1993

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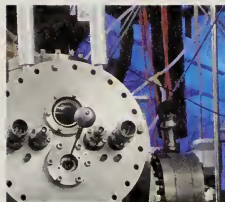
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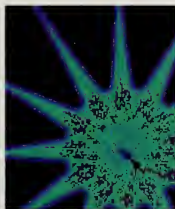
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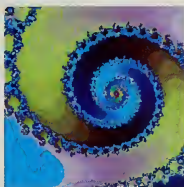
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See inside back cover for details on
anonymous FTP, Gopher, and World
Wide Web.

HPCC AND ENGINEERING

"Power and Progress in the Mechanical Age" was painted in 1939—at the threshold of World War II. Once again the entire globe is in a state of transition with the ending of the Cold War. As we momentarily poise to meet whatever challenges await, scientists and engineers anticipate new needs. Just as in the Mechanical Age, engineering will be a major player.

Some "hot" innovations in the experimental aspects of engineering, such as nanolithography (see page 4) and multimedia in the laboratory (page 10), are just two examples of the current generation's technological advancements. Computational mechanics (see page 12) offers further potential.

Today's world is keenly aware of the environment, and high-performance computing is providing solutions. Through its unique capabilities in processing large datasets, HPCC aids in the development of more efficient engines (page 8) and in the understanding of the Earth's complex systems (pages 20 and 21).

Virtual reality, a 21st century technology, is being employed by award-winning design engineers at Caterpillar, an NCSA industrial partner, to develop better field machines (page 24). Advancements in XUNET, a bridge to implementing the information highway, are described on page 26.

NCSA is enabling students to learn real science via networking and special software (page 27). A new section, "new technology" (pages 30–33), begins in this issue. Additions to NCSA's resources, including new hardware and software, will be featured in this department.

Other news follows in "center activities." —*Fran Bond, Editor*



*"A nation is never finished.
... It has to be recreated
for each new generation."*

—John Gardner

"Power and Progress in the Mechanical Age" painted by Bettie Becker and Frank Wiater, two seniors in Art and Design at UIUC, under the supervision of Professor Warren Doolittle (1939) is a mural on the first landing of the East entrance to Talbot Lab, Engineering campus, UIUC. (Photo by Wilmer Zehr)

by Randall Graham, Science Writer

DEVELOPING

"When it comes to making faster, smaller computers, the microelectronics industry is reaching a limit," says Joseph Lyding, NCSA principal investigator and UIUC professor of electrical and computer engineering. "Our goal is to use the Scanning Tunneling Electron Microscope (STM) for research—particularly in the area of circuit miniaturization."

STM defined

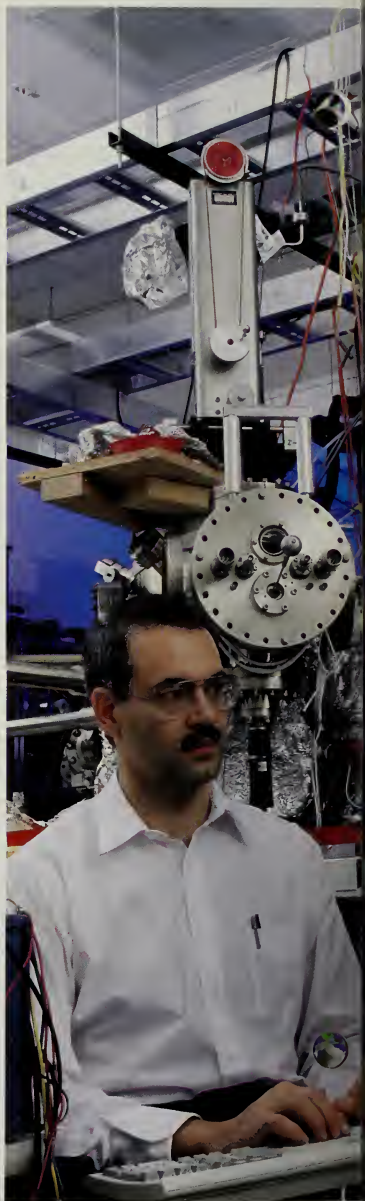
STM is one of two types of 3D atomic resolution microscopes. The other is the Atomic Force Microscope, or AFM, which generates images by measuring the atomic forces of interaction between its scanning tip and the sample's surface atoms. (A number of UIUC faculty are planning to utilize an AFM facility that is being established at the Beckman Institute.) Only STM, however, allows scientists to study both topographical and electrical properties of materials, which are important for understanding the behavior of microelectronic devices. STM is also the only instrument with the ability to rip atoms from the sample surface and relocate or otherwise manipulate them.

TOOLS FOR

Lyding's STM produces atomic-scale pictures by positioning its sharp tip a few atomic diameters from the sample and raster-scanning it to produce an image. Just enough voltage is applied to the tip to cause a small quantum mechanical tunneling current to jump across the gap to or from the sample. The quantum mechanical tunneling current (which cannot be explained by classical physics) is exponentially dependent on the distance from the tip to the atomic surface, so that one can convert tunneling current to the tip height above the surface very accurately.

As the tip scans, the electrical and topographic properties of the atoms in the sample cause variations in the current. A feedback circuit moves the tip normal to the surface to minimize current variations. The feedback information is then processed into a picture on the atomic scale. Increasing the voltage enables a researcher to move atoms around, pile them up, or trigger chemical reactions. This activity takes place in an infinitesimal world of invisible units.

NANOLITHOGRAPHY



nano-lithog-ra-phy is a technique used for integrated circuit fabrication done on a dwarfed scale. (The prefix *nano* represents 10^{-9} , or one-billionth of the unit adjoined.)



"Current resolution with optical nanolithographic techniques is on the order of a half micron, about 5,000 angstroms," Lyding says. "Those methods are expected to hit their limit at around 1,000 to 2,000 angstroms in the next ten years. This is due to the wavelength restriction of the UV [ultraviolet] light used to project the circuit image onto a chip.

"STM can easily make devices in the sub-1,000 angstrom resolution range. Recently we have used it to chemically modify silicon surfaces with 20 angstrom resolution. In these experiments, electrons from the STM tip are used to trigger local chemical reactions between the surface and adsorbed gas molecules."

Joining UIUC

Lyding built his first STM personally, turning the parts in a UIUC machine shop. He holds a patent on one microscope currently being sold and has designed a nonmechanical method of positioning samples to eliminate vibration problems. "You can actually pick up my microscope while it's scanning, and the sample and tip will not crash into each other," he says. Lyding's STM, and other designs based on it, are widely used. Because of its simplicity, he explains, most users build their own instead of buying commercial products.

In 1984 Lyding came to the UIUC to study the dynamics of charge-density wave (CDW) transport in quasi-1D metals, under the tutelage of electrical and computer engineering Professor John Tucker and legendary two-time Nobel physicist John Bardeen. While using STM to observe CDWs, Lyding became fascinated with the technology's endless experimental possibilities.

"John Bardeen encouraged my pursuit of STM," says Lyding. "He was very interested in probing the microscopic aspects of CDW phenomena, and he also encouraged the semiconductor STM work that we are now pursuing."

Nanolithography continued on page 6

"All of this interactivity between machines is transparent to the user, thus . . . I can concentrate on the experiment," says Joseph Lyding, shown here with his lab setup in the Beckman Institute. Seated before the HP 700 workstation, he calls up an AVS file of an experiment that was run on NCSA's CONVEX C3880. STMs are housed in vacuum chambers in the background. (Photo by Wilmer Zehr)



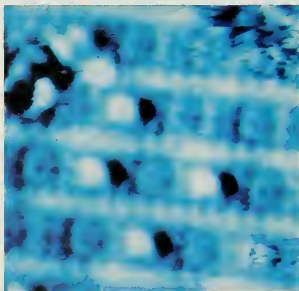


Metacomputing at NCSA

"I'm always looking for ways to mechanize things," Lyding adds. To him, an alliance with NCSA seemed perfectly natural. "NCSA has given me the ability to control my lab from remote locations while viewing real-time images from the microscope. This means that once my students learn how to run the microscope, they can run it from anywhere."

Key to Lyding is the integration of the STM experiment into NCSA's metacomputer environment [see *access*, September–December 1991]. Since Lyding's STM facility is located in the Beckman Institute, which is intended to intermingle various scientific disciplines and to encourage collaboration, it was inevitable that he would learn of NCSA and its biological imaging group headed by Clint Potter.

"A typical scenario for us is to use AVS [software] in conjunction with NCSA's CONVEX C3880 and CM-5, and our laboratory's HP 700 [Hewlett Packard] and PCs simultaneously. We typically use Rachael's [NCSA research programmer Rachael Brady of the biological imaging group] STM module running on the CONVEX to control the STM, acquire image data, and perform Viewit operations. [Viewit is a general-purpose software for manipulating multidimensional arrays. It was developed by Potter and his group in collaboration with the Biomedical Resonance Laboratory.] All of this occurs within a



remote module from within AVS, which is running on the HP in our laboratory. AVS on the HP is used to render high-quality light-sourced images of the STM scan area, bringing out details that we cannot see in the raw data.

"Furthermore, we frequently process these images by taking 2D fast Fourier transforms [FFT] and looking at the power spectra for symmetry features in the image. The FFT module in our HP-AVS display actually sends the data to the CM-5 for parallel computation of the power spectrum which is then displayed on the HP.

"All of this interactivity between machines is transparent to the user, thus my students and I can concentrate on the experiment and use the advanced rendering and analysis to steer the course of the experiment."



SIGGRAPH demo

Lyding demonstrated his metacomputing capabilities at SIGGRAPH '92 in Chicago as part of the innovative Showcase. Funded by NSF and ARPA, Showcase was the largest exhibit and featured 40 interactive and collaborative leading-edge applications of HPCC. It was supported by fourteen corporations and six forefront laboratories [see *access*, May–June 1992].

An SGI workstation in a Showcase display booth was connected to NCSA's CONVEX C3880 in Urbana via the T3 fiber optic link. "People were genuinely impressed when they found out we were controlling a live experiment from Urbana in Chicago and could remotely move the STM scan area around in real time," says Lyding. "The distance had no effect on response time."

Providing Lyding with remote capabilities was a challenge for Brady, who explains how she forced a solution: "All of Joe Lyding's microscopes are controlled by IBM PCs running MS/DOS on either 386 or 486 chips. These are single tasking machines, which means you cannot run something in the background while you do something in the foreground. To hook his computers up to

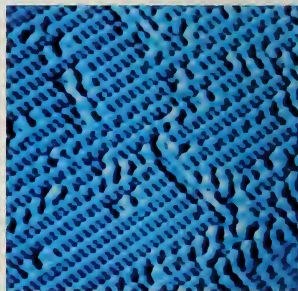
another box, those PCs are going to have to control the experiment and at the same time listen on the network for any commands coming from a remote site.

"Making his machines do two things at once is a total hack. You tie all the network listening stuff to interrupts, which are built into the MS/DOS operating system. When a request comes from the network, it gets shoved into a buffer on the PC and a flag is set within the PC's hardware. . . . Right now, this is all done synchronously. Next, we would like to do it asynchronously—that is, interrupt Joe's program and say 'here's a new request.'"



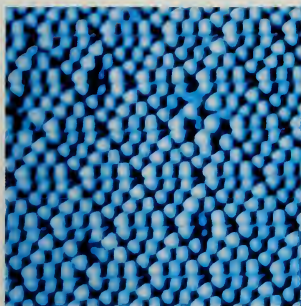
More power for micromanipulation

The STM's ability to manipulate atoms has Lyding and others considering it for microelectronic manufacturing roles. To advance this effort, Lyding joined six colleagues from UIUC and two from the University of Minnesota in founding the STM-based Nanolithography University Research Initiative. They study the behavior of proposed new electronic devices and design STM techniques for fabricating them.



(Far left) GaAs (100)—gallium arsenide—showing as atoms in channels on surface. (Above right) Si (100)—silicon—surface showing dimer rows of Si atoms.

(Courtesy of Joseph Lyding)



*"I'm always looking
for ways to mechanize
things."*

—Joseph Lyding

full quantum mechanical molecular dynamics simulation of the tip and surface atoms in response to the fields and forces that exist in the tunneling junction," says Lyding. "Tremendous compute power is needed to extend this calculation to a volume consisting of, say, 50 atoms that might realistically bound the volume of tip/surface interaction. This effort will dovetail smoothly with the existing compute/experiment protocols developed for us by NCSA.

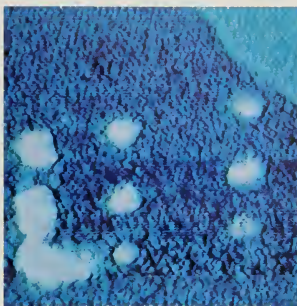
"Hess has proposed a number of intriguing new electronic devices that will only operate in the size regime where quantum effects emerge and dominate," Lyding continues. "Using conventional lithographic technology, these devices will only work at liquid helium temperature (4.2 K) or lower. However, with STM nanolithography, room temperature operation should be possible. Hess is working in close collaboration with Tucker on developing and simulating new device concepts that are amenable to STM nanolithography."



Linking with other scientists

"I think there are a lot of other scientists out there who could benefit by networking their scientific instruments with NCSA's machines," says Brady. "It's just that they do not realize the potential advantage when they have been getting by without us."

In September, Brady got an opportunity to outreach to other researchers when she copresented with Lyding at the Workshop on Real-Time Applications of High Performance Computing for Biological Imaging that NCSA cosponsored



(Far left) Si (111)—silicon—surface showing detailed atomic structure. (Above right) "UI" written with small piles of silicon atoms on a Si (111) surface. Atoms were moved by the STM.

AVS running on NCSA's CONVEX C3880 was used to control Joseph Lyding's STM nanolithography experiment in which "NCSA" was written on a silicon surface that is shown above each head on this spread. (Courtesy of Joseph Lyding)

with the Beckman Institute with NSF funding. Their topic was entitled "The Distributed Scanning Tunneling Microscopy Laboratory: Real-time Control, Visualization, and Modification at the Atomic Level." Potter and Bridget Carragher, director of the Optical Visualization Facility at the Beckman Institute, were co-chairs.

"The great thing about working with Joe is that he appreciates computers," says Brady. "He understands what they can do." ▲

NOTE: If you want to order a videotape about Lyding's research, "A Quantum View" from NCSA RealTime #4, contact Orders for Publications, NCSA Software, and Multimedia [see [ncsa contacts](#), page 2].

UIUC members of the research group include: Ilesanmi Adesida, Stephen Bishop, K.-Y. (Norman) Cheng, Karl Hess, and John Tucker, Department of Electrical and Computer Engineering, and Munir Nayfeh, Physics. Members at Minnesota are Stephen Campbell and Ted Higman, Department of Electrical Engineering.

"We are finding that these tiny new devices will not function like today's larger-scale ones. Quantum mechanical effects begin to play a dominant role, so we are exploring ways to harness those effects for our advantage."

Since STMs operate sequentially, a large array of them will be necessary to map circuits with enough speed to be cost effective. Lyding's STM images are currently rendered from 2D datasets, but they will become 3D as soon as he begins to use electron energy as the third dimension.

Lyding says he will need teraflops computing speed to bring detailed simulation of the tunneling probe tip and its interaction with the sample online with the experiment. Understanding the probe tip is especially important in the STM-based Nanolithography University Research Initiative where atomic-scale surface modification schemes are being developed. Voltages required to modify a sample could also damage the tip.

Other collaborations underway with Karl Hess, director of the NSF-funded National Center for Computational Electronics (NCCE), will also require more compute power. "Karl Hess's group has developed the analysis tools to perform a

Vehicle manufacturers are finding themselves in a quandary: the 1990 amendments to the Clean Air Act require considerable reductions of pollutant-forming emissions by the year 2000, and there is ever-increasing pressure to improve fuel efficiency. At the same time, competitive market pressures demand a faster turnaround time for new designs than ever before. Fortunately, vehicle manufacturers have some new tools to help them keep pace with the demands of the environment and the market. One of them is engine modeling, or the creation of a "numerical engine"—allowing manufacturers to test new engine components on computer before creating expensive prototypes.

Dennis Assanis, associate professor in the UIUC Department of Mechanical and Industrial Engineering, has been performing pioneering work modeling turbulent flows in engines

to tailor his research efforts to the problems and challenges faced by the automotive industry.

Modeling turbulent reactive flows

Internal combustion engines are extremely complex energy systems, involving the coupled phenomena of combustion, turbulent fluid flow, turbulent flame propagation, ignition and extinction, pollutant formation, and wall heat transfer, and in diesel and fuel injection engines, spray dynamics. Those phenomena are characterized by a number of different time and length scales. Because of the extreme computational demands, engine combustion modeling has been identified as a Grand Challenge problem.

One of the most powerful multi-dimensional engine simulation codes

internal combustion engines, Assanis and his students at UIUC found that it does not adequately predict some aspects of fuel spray dynamics and pollutant formation. Their improvements are being incorporated into a new version of KIVA called KIVA-3. Unlike KIVA-II, KIVA-3 can handle both the intake and exhaust flows, allowing for the simulation of an entire cycle.

In automobile engines prior to the mid-1980s, air and fuel were mixed in a carburetor prior to entry into the combustion chamber. In modern gasoline engines, fuel is sprayed into the ports of individual cylinders. In diesel engines, fuel is sprayed directly into the combustion chamber. The formation and dynamics of a fuel spray—poorly understood from a

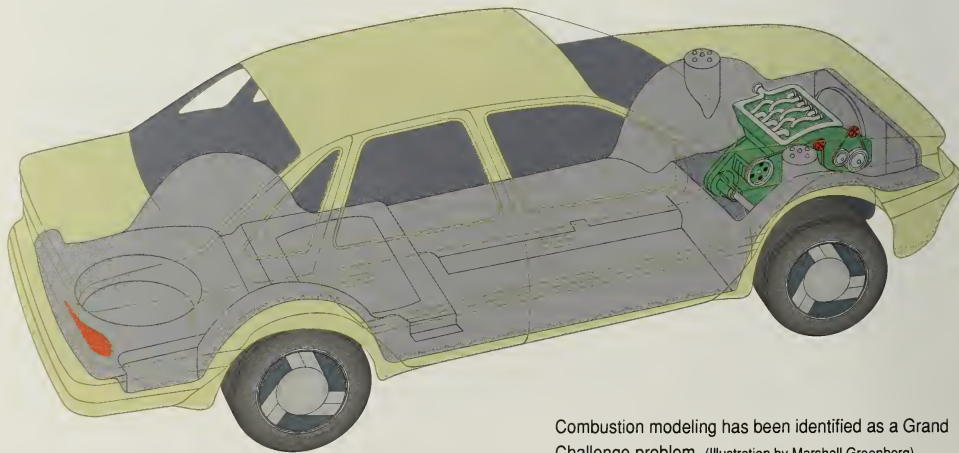
Creating the numerical engine

by Sara Latta, Science Writer

on NCSA's high-performance computers. He spent part of his 1991-92 sabbatical at NCSA, working to improve engine modeling techniques, and part of it traveling to major vehicle manufacturers worldwide. Assanis wanted

is KIVA and its offshoot, KIVA-II, developed by the Los Alamos National Laboratory (LANL). Although KIVA-II, a vectorized code for Cray super-computer systems, can deal with many of the phenomena occurring in

modeling or experimental standpoint—is crucial to the combustion process. The droplets must be small enough to evaporate readily so as to mix with the air—within flammability limits. Assanis is trying to add to KIVA-3 much of the knowledge about single-drop evaporation under high temperatures and pressures into the reality of drop evaporation in a spray.



Combustion modeling has been identified as a Grand Challenge problem. (Illustration by Marshall Greenberg)

Unless the combustion chamber is very large (as it is in some diesel engines), some of the fuel spray will impinge on the walls of the chamber. "We do not really know what will happen after the droplets impinge upon the walls," says Assanis. "They can shatter into smaller droplets, they can rebound from the walls, or they can form fuel films on the walls, which may then evaporate. Depending on what happens to the droplets after impingement, fuel mixing can be better or worse." KIVA-II assumed that drops reaching the wall stick to the wall and continue to vaporize.

Assanis has incorporated other impingement options into KIVA-3,

device), and how to improve the mixing and penetration of the gaseous fuel plume with the rest of the air in the combustion chambers."

Improving total system design

Assanis found—during his sabbatical tour of automobile manufacturers in Europe, Japan, and the U.S.—that although KIVA-II is among the software of choice in the companies' research labs, it is still not used for real engine design.

"I don't see KIVA being routinely used for component and system

merical engine

producing a code that is much better at predicting the actual behavior of the fuel droplets.

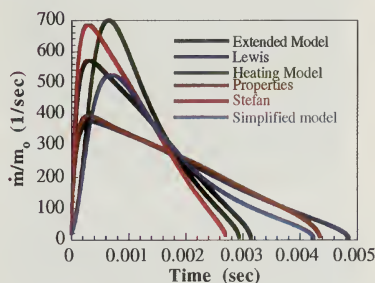
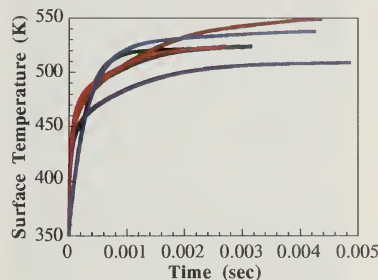
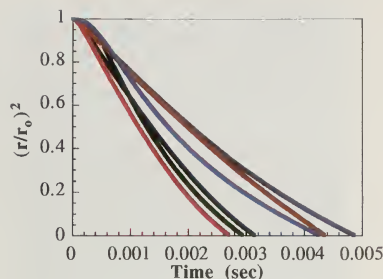
During the combustion process, fuel vapor can be absorbed on the thin layer of oil present on the walls of the combustion chamber. Later in the cycle, as temperatures drop, the fuel vapor is released back into the chamber—just in time for the exhaust process. According to Assanis, this is one of the major mechanisms leading to unburned hydrocarbon emissions—major culprits in pollutant formation. Assanis is using KIVA-3 to better model this behavior, an area of which he says: "I feel that we are pioneers."

Assanis is currently working on improving KIVA-3 to model direct injection of natural gas into the combustion chamber. In the near future, he hopes to collaborate with experimentalists to validate code predictions. "Lately, people have started to realize that natural gas is a fuel with great promise in terms of reducing pollution and improving fuel economy," says Assanis. "This presents a new challenge. We would like to be able to provide some guidance to industry on how to improve the design of gaseous fuel injectors, how to position and target them, where to place the glow plug (an ignition assist

design for at least another ten years," he says. Modeling all the complex processes inside the combustion chamber means little if engine designers are unable to interpret and couple those processes with other engine components. Yet the results of these computational fluid dynamics (CFD) computations are not readily interpretable by most designers.

Assanis is taking the results from KIVA and incorporating them into thermal, structural, and other systems level codes, in an attempt to bridge the gap between modeling and actual design and manufacturing. Working with NCSA's Software Development Group, Assanis hopes to create visualizations and animations of fluid and spray dynamics and their interactions, an approach that he feels will allow designers to better understand the results of the KIVA code.

Another problem is that a typical simulation of just one cycle takes about 30 hours on the CRAY Y-MP system, a time that Assanis says is simply unacceptable to industry designers. Advances in rapid prototyping have allowed designers to cheaply test some—but not all—components. He says many medium-



Evaporation history of a decane droplet, initially at a temperature of 350 K, injected into air at a temperature of 1000 K and a pressure of 10 atmospheres. Computations using the model proposed by Varnavas and Assanis (black lines) are compared with other simplified droplet evaporation models, including one in the original KIVA code (blue lines). (Courtesy of Constantine Varnavas and Dennis Assanis)

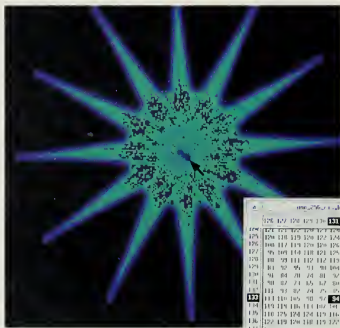
Engine continued on page 19

Engineering



The 1988 crash of United Airlines Flight 232 in Sioux City, IA, might have been prevented if the computer-aided tomography (CAT) scan data and visual analysis techniques used by Ron Kriz and his collaborators at NASA Langley had been available. The cause of the crash was a crack in a turbine fan blade in the aircraft's engine—a flaw not always detectable by conventional ultrasonic non-destructive testing.

Kriz, NCSA's academic affiliate representative from Virginia Polytechnic Institute and State University (Virginia Tech), came to Champaign-Urbana in the summer of 1992 with a set of data supplied by the manufacturer of QUEST, a CAT-scan system that detects small flaws in advanced material systems. Using NCSA's visualization software (i.e., X DataSlice Isosurface, Viewit, X DataSlice Dicer, and X Image), Kriz transformed the complex dataset into an image of a turbine fan blade—with a serious flaw hidden in the center (see image above left). The results of his visual analysis efforts helped Kriz secure a contract with NASA Langley Laboratory, which had just acquired a QUEST system of their own for materials analysis.



Building the lab

An associate professor of engineering science and mechanics, Kriz has become something of the "visual analysis guru" in Blacksburg, VA. Beginning in 1990 with just a couple of Sun SPARC 2 workstations and PV Wave software, he and his colleagues soon realized the need for a more comprehensive visual analysis lab.

With the financial backing of the High Performance Polymers and Adhesives NSF Science and Technology Center and the Virginia Institute for Material Systems, and space from his department, Kriz formed the Scientific Visual Analysis Laboratory at Virginia Tech. The facility, which is open to any Virginia Tech faculty member, is equipped with two Macintosh IIx computers with multimedia capabilities, two Sun SPARC 1

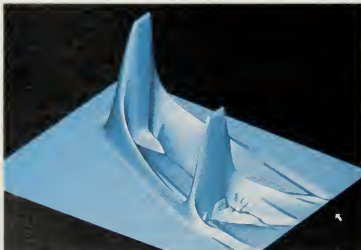
workstations, two Sun SPARC 2 workstations, and one Silicon Graphics IRIS-4D/320 VGX system. Most of the lab's software programs are from NCSA's Scientific Visualization Software Suite produced by the Software Development Group (SDG). All these efforts led Digital Equipment Corporation to start a digital visualization reference center in the visual analysis lab.

"After building the laboratory," says Kriz, "I returned to NCSA to learn how to use the visual analysis tools. The support I received from the folks at NCSA, especially those in Joe Hardin's [SDG] group, was really fantastic. There was hardly any learning curve at all, which translated back to my students and colleagues at Virginia Tech. As an academic affiliate representative of NCSA, I can provide the people working in the laboratory a choice of computers and software."

Kriz has brought NCSA's visual analysis tools to the classroom as well. He created a new course in scientific visual analysis, during the same busy summer that he put together the Visual Analysis Lab, and came to NCSA to learn to use visualization tools. Students in the course, popular among engineering students in a number of areas, develop projects in scientific visual analysis that culminate in multimedia presentations.

"This eventually helped to support the creation of a new multimedia laboratory for undergraduate education," says Kriz, "as part of the NSF SUCCEED program." Virginia Tech is one of eight southeastern universities that comprise SUCCEED (Southeastern University and College Coalition for Engineering Education). "We're anticipating that we will be using NCSA sonification tools [see *access*, May-June 1991] in our multimedia lab," Kriz continues. "The director of that lab, Gordon G. Miller III, is interested in using NCSA visualization tools, like Image and DataScope, in the lab."

During the summer of 1993, three undergraduate students worked with



Visualizations on this spread (counterclockwise from top of page 10) show profile of a titanium turbine, flaws (black spots) in a turbine cross section, and a sequence of wave propagation in an epoxy/graphite composite. The latter is a unipolar-planar pulse that can only be created with a supercomputer. (Courtesy Ron Kriz)

their professors at Virginia Tech to develop multimedia training modules for undergraduate courses in chemistry, materials science, and engineering science and mechanics. Funding was provided by the NSF Science and Technology Center Summer Research Undergraduate Program. Virginia Tech has an anonymous ftp site to distribute the multimedia modules, which are specifically geared to engineering students. Enter `ftp viz2.multimedia.vt.edu` to obtain these modules. Username is `anonymous`; password is `E-mail`.

Multimedia applications are deemed so important to the College of Engineering's curriculum that this fall's freshman class is required to have computers that can handle

"The support I received from the folks at NCSA . . . was really fantastic."

—Ron Kriz

multimedia applications such as animation, graphics, photographs, full-motion video, and sound. For nearly a decade, the college has required students to have their own computers.

"Seeing" stress wave measurements

Having performed some preliminary simulations and visualizations of acoustic microscope measurements on MIT's CRAY-2 system, Kriz now plans to use Thinking Machines' CM-5 system at NCSA to do the same.

An acoustic microscope differs from an optical microscope in that it uses stress waves (sound waves traveling through a solid material), rather than light waves. "Stress waves do not just reflect off the surface of a material," says Kriz. "They penetrate and can reflect off structures below the surface as well.

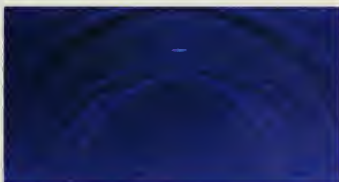
"The materials I am studying—fiber-reinforced epoxy polymers—have fibers below an epoxy polymer surface. The area where the fibers bond to the polymer forms an interphase—not a fiber, not a polymer, but something in-between."

Kriz plans to use NCSA's CM-5 to simulate the propagation of stress waves below the surface of the polymer and the reflection off the fibers below. After running the simulation and visualizing the nature of the interphase, Kriz can better interpret the actual measurements from the acoustic microscope.

"This is the first time," Kriz adds, "that anyone has ever experimentally measured these interphase structures by stress wave propagation. The objective is to bring the two—simulation and visualization, and experimental measurement—together. We're getting there." ▲

NOTE: Virginia Tech's Visual Analysis Lab has posted material on its Gopher server. Using NCSA Mosaic, select the NCSA Mosaic Home Page, then World Wide Web; W3 servers; Virginia Tech (under Virginia); Visualization Lab.

For directions about obtaining NCSA-developed software, see the inside back cover.



Ron Kriz

with *by Sara Latta, Science Writer*

Visual Analysis

NCSA and

Structural Mechanics

by Jarrett Cohen, Staff Associate, Director's Office

"Our goal is doing computational mechanics, especially solid mechanics, on massively parallel machines," says M. Fouad Ahmad, NCSA research scientist in structural mechanics.

Ahmad, who holds a Ph.D. in theoretical and applied mechanics, is collaborating with researchers from several engineering disciplines in academia and industry. A large part of Ahmad's time is spent in helping researchers better use NCSA's resources for the structural mechanics community. Some examples follow.

Analysis of shear flow localization

Tarek Shawki, UIUC associate professor of theoretical and applied mechanics, is pleased with the outcome of his collaboration with Ahmad on shear flow localization. Their results, Shawki says, put "things into a form that is easily used by the engineering community."

Beginning with his graduate studies at Brown University in the early 1980s, Shawki has been studying the phenomenon of shear flow localization—"a mechanism through which materials fail to carry the load they are supposed to carry."

Localization takes place "by the concentration of plastic deformation into narrow, band-like regions instead of being uniformly spread out," he says. It occurs in such applications as projectile impact, high-speed machining, high-speed cutting, and armor penetration.

Conditions that lead to shear flow localization are numerous, which is what makes the problem so complex, according to Shawki. Material behavior, rates of deformation, inertia, heat conduction, and boundary conditions are just a few.

Shawki's research involves both analysis and computation. On the analytical side, he and his colleagues have developed nonlinear solutions for special cases and a new "energy-based localization theory."

"The energy-based theory associates localization with a characteristic evolutionary behavior of the system's total kinetic energy," says Shawki. "In this context, the kinetic energy plays a fundamental role as a single parameter capable of characterizing the complete localization history."

"With that discovery," he continues, "we realized that computations that have been performed in the past were not always covering the full localization history. What we saw on the computer was not what we expected through the theory. Armed with the theory, we realized that we could push the computations a lot further."

New performance levels

"For a computation to resolve the evolution of localization until failure takes place," Shawki stresses, "great care should be taken to ensure that the numerical scheme converges to the right answer." Even though the physical event takes place within microseconds or milliseconds, getting to the final stage of localization is computationally demanding, he adds.

First attempts by Shawki and NCSA research assistant Harischandra Cherukuri to reach the "right answer" involved running 1000 x 1000 grids for five days straight on a Hewlett-Packard 750 workstation. About two years ago, Ahmad joined their team. His first step was to optimize the code for the CRAY Y-MP system, achieving 130 MFLOPS on a single processor.

"Our goal is doing computational mechanics, especially solid mechanics, on massively parallel machines."

—M. Fouad Ahmad

After further investigation of the motion and energy balance equations that depict localization, Ahmad says "it seemed quite obvious that they could be parallelized." He went on to rework the code for NCSA's CM-2 and then the CM-5 systems (both from Thinking Machines Corp.). On the CM-5's full 512 nodes, the code ran at 11 Gflops for a very fine grid. (See graph on page 13 for Mflops rates on several machines.)

"Today, problems which took days to solve before take less than six hours on the CM-5," Ahmad says.

This simulation mirrors and agrees with the results of an experiment done at Brown University, Shawki says. "It is a model for a Kolsky bar experiment, which involves applying a torque at a high rate to a thin-walled tube."

The NCSA/UIUC team used AVS for their visualization software, with data moved from the CM-5 to the CONVEX C3880 system. Daniel Cancro, an undergraduate intern at NCSA on leave from the University of Notre Dame, wrote the AVS module to interpret the data.

The visualization was part of a videotape "A Massive Parallel Computation of Plastic Flow Localization in Dynamic Viscoplasticity." The video shows a solid block, subject to continued shearing, that appears to break into two rigid blocks. A small colored band between the blocks represents the localized zone. Color designates where significant temperature increases occur.

"The material inside those localization regions softens as the temperature increases, and it deforms more," Shawki says. "As it deforms, it generates heat, and that heat contributes to further softening, and the cycle continues, leading to further localization. It is catalytic."

"The final catastrophic behavior has not been reported before; the visualization shows the details of the temperature rise and the deformation," Ahmad adds.

A Grand Challenge

This "very careful development of the numerical schemes led to results that really exhibit the same things that the theory anticipated," Shawki says. "With recent advances involving the energy characterizations, it appears that the kinetic energy is a potential candidate for the characterization of localization."

Even with an 85-fold increase in speed over the Y-MP on the CM-5, today's machines are not powerful enough to make a definite determination, classifying this as a Grand Challenge project. The current study only considers one spatial dimension. "A higher dimension, even at this speed, would take thousands of hours on a CM-5," Ahmad says.

This difficulty is caused by the need for a very fine grid, which Ahmad calls a "Catch-22," as a finer grid requires more timesteps. The current 1D simulation already takes 3 million timesteps. Since teraflop computers are expected to be available by the mid-1990s, such hurdles will not remain insurmountable for long.

With such performance in hand, Shawki hopes "this energy development leads us to the identification of a material resistance to localization that can be experimentally measured and tabulated in materials handbooks."

Ahmad presented this work at the First Computational Mechanics Working Group Meeting of the National Consortium for High Performance Computing (NCHPC), held May 19-20 in Albuquerque, NM. Engineers from universities, industry, and government attended. One of the workshop's purposes was facilitating collaborations between NCHPC members and industry in HPCC use, a task with which Ahmad is much engaged.

Other ongoing academic projects in which Ahmad is involved include the study of viscoelastic material with Harry Hilton, UIUC professor emeritus of aeronautical and astronautical engineering, and the probing of the micromechanics of composite materials with Rami Hajali, UIUC graduate student in civil engineering.

Helping businesses

Besides working with the academic community, Ahmad aids companies in their R&D efforts. Structural mechanics projects with Caterpillar, an NCSA industrial partner, have involved simulations of waste properties in landfill compaction and of the edge-rolling process for equipment design. With Dow, the effect of foam structure on cushioning properties of flexible polyurethane was modeled.

In the last year, Ahmad also worked with a smaller company, Bonutti Orthopedic Services, Effingham, IL,

whose research was funded by the Illinois Consortium for Technology Transfer [see *access*, January-February 1991]. Forty-five employees work in the Bonutti complex, which includes a clinic; a sports medicine and physical therapy area; and Apogee Medical Products, the R&D arm.

Developing orthopedic devices

James Hawkins, R&D director at Apogee, says the company's philosophy is that "all aspects of a person's wellness are incorporated into the group." Founder and president Peter Bonutti is an orthopedic surgeon. "When Dr. Bonutti is performing surgery, he sees the need for new devices to help him," says Hawkins. "Apogee was begun for R&D because he had special applications."

Treating Carpal Tunnel Syndrome is one example of a special application. In operations, Bonutti needs to "create a potential space in the wrist [and] . . . to incrementally expand tissue in a defined area," Hawkins says. To do this, it is necessary to "know the size and shape of the space that the expander would create."

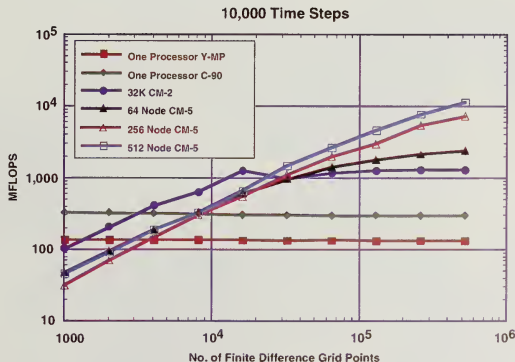
To model expander shapes, the company turned to NCSA for assistance. In the summer of 1992, Hawkins began a collaboration with Ahmad and NCSA research assistant Gerry Pollock, a recent Ph.D. graduate from UIUC in aeronautical and astronautical engineering.

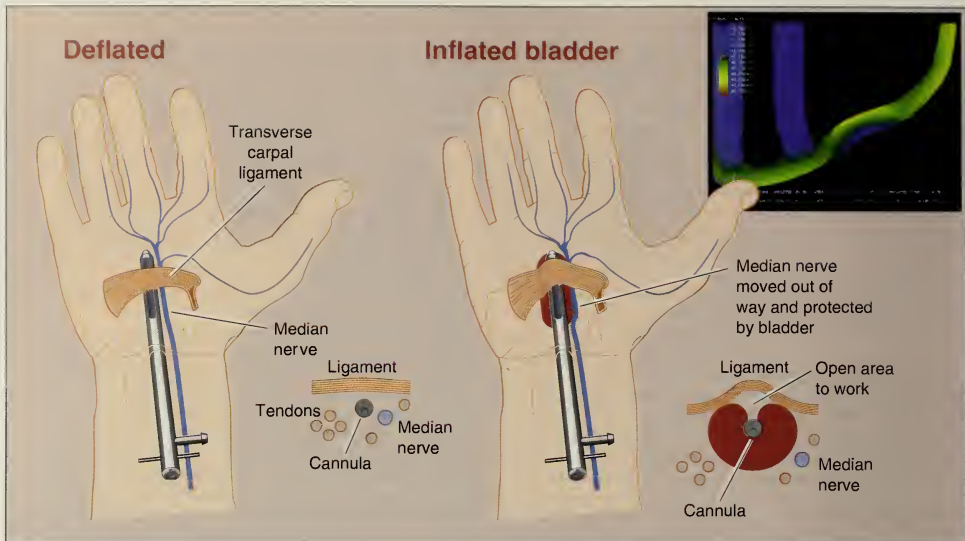
NCSA initially trained Hawkins on the center's systems. For the expander project, he used the CRAY-2 system from a Silicon Graphics workstation at NCSA.

The expander "pushes flesh out of the way so they can see the area a little better. They insert a camera through the hollow center," Pollock says. Bonutti had been using mechanical devices but wanted to try a balloon instead, he explains. "He wanted to follow the same procedures but in a way that the tissue would be less damaged."

Structural mechanics continued on page 14

Mflops rate for different machines. As an extension of his collaboration with Tarek Shawki, M. Fouad Ahmad is studying the performance of the shear flow localization code on several platforms. Mflops performance rates are given for a 10,000 timestep simulation. (Courtesy M. Fouad Ahmad and Tarek Shawki)





Structural mechanics continued from page 13

Modeling expanders

Employing finite element analysis, the NCSA and Apogee collaborators looked at several different shapes. "Initially, we had hoped to effectively predict the shape of an expanded balloon from its deflated geometry and its material properties," Hawkins says.

To accomplish this goal, they employed an iterative technique. It takes a large amount of computer time to expand the balloons, since it is done incrementally. "The expander is a nonlinear problem; access to supercomputers is important," Pollock says. "On a workstation, it would take a couple of days."

After completing the supercomputer models, Hawkins and his team at Apogee tried several experimental designs in the laboratory—principally to solve material inconsistencies. "By theoretically performing the design iterations on the computer, we save a great deal of time and money."

Creating better knee replacements

A more recent Apogee project is *patella*, or kneecap, replacements. Pollock says they are typically made of a laminate, with a polyethylene part in contact with the tissue and a metallic part that meshes into the bone.

Hawkins says the patella replacement is applied using a solid layer of cement—which Bonutti wants to avoid. "We looked at using smaller amounts of bone cement," he says. "We are trying to see if it will have the same fixation strength. Our related research indicates that less cement is better."

Again taking a finite elements approach, the team modeled several patella designs with "loading" on them and evaluated the stress distribution through the system. Loading is the stress put on the knee by a bent leg, for example, when climbing stairs.

Treatment for Carpal Tunnel Syndrome with expanders developed using NCSA's computational resources.

(Illustration by Marshall Greenberg)

Inset: Expansion of bladder cross section with uniform internal pressure. (Courtesy Peter Bonutti)

This computational analysis looked at new geometries and less cement as opposed to a solid layer of cement. The models were carried out on NCSA's CRAY Y-MP system, with visualizations created using a postprocessor.

"After the computer modeling, we created geometries like the model to see if what the computer said actually happens," Hawkins says. The patella replacement work will be useful for studying other cemented components.

New applications code

As part of Ahmad's responsibilities to NCSA users in structural mechanics, he enables them to have state-of-the-art resources, such as software. Recently he and NCSA research programmer Danesh Tafti got Centrex Spectrum

software application for fluids and solids on the CRAY Y-MP system. Soon a CM-5 version will be in place. According to Ahmad, it is a "new code with great potential." ▲



M. Fouad Ahmad
(photo by Thompson
McClellan Photography)

Allocations in engineering

- Suresh K. Aggarwal**, UIUC, "Computations of Particle-Laden Turbulent Flows" and "Comprehensive Modeling of Multicomponent Fuel Sprays"
- Russell L. Alberts**, U. of Nebraska, Lincoln, "Finite Element Analysis of Retained and Removed Orthopedic Screws and Finite Element Analysis of the Growth Plate in Bone"
- Ryoichi S. Amano**, U. of Wisconsin, Milwaukee, "Computations of 3D Turbulent Flows in Gas Turbines"
- Ronald Paul Andres**, Purdue U., "Molecular Dynamics Simulations of Cluster Melting, Cluster-Cluster Collisions, and Cluster-Substrate Interactions"
- Mehdi Anwar**, U. of Connecticut, "Transport in Lower Dimensional Structures"
- Dennis N. Assanis**, UIUC, "Development of an Improved Evaporation Model for the KIVA-3 Multidimensional Engine Simulation"
- Nasser Ashgriz**, SUNY, Buffalo, "Numerical Simulation of Binary Drop Collisions"
- S. Balachandrar**, UIUC, "Simulation of High Rayleigh Number Thermal Convection with Imposed Mean Shear and System Rotation"
- Constantine Balanis**, Arizona State U., "Finite-Difference Time-Domain Technique for Antenna Radiation"
- Sanjoy Banerjee**, U. of California, Santa Barbara, "Multiphase and Interfacial Phenomena"
- Romesh C. Batra**, U. of Missouri, Rolla, "Studies in Penetration Mechanics"
- Yildiz Bayazitoglu**, Rice U., "A 3D Model for the Enhancement of Heat and Mass Transfer from a Sphere in a Superimposed Acoustic Field"
- Robert A. Beddini**, UIUC, "Simulation of Large-Eddy Turbulence in Compressible Ducted Flows"
- Theodore B. Belytschko**, Northwestern U., "Adaptive Multidomain Methods for High Gradient Problems in Solid Mechanics"
- Lawrence Alan Bergman**, UIUC, "Solution of the Fokker-Planck Equation Arising in Stochastic Dynamical Systems"
- M. A. Bhatti**, U. of Iowa, "Performance of Rigid Concrete Pavements Subjected to Dynamic Vehicle Loads"
- Amir Boag**, UIUC, "Complex Multipole Beam Approach to Electromagnetic Scattering"
- David E. Boyce**, UIUC, "Dynamic Route Guidance Systems Design" and "Transportation Network Equilibrium Modeling"
- M. Quinn Brewster**, UIUC, "Nonsteady Burning of Solid Fuels in the Presence of Thermal Radiation and Pressure Transients" and "Solid Rocket Motor Internal Flowfields"
- Richard O. Buckius**, UIUC, "Rigorous Predictions of the Scattering of Thermal Radiation from Very Rough Surfaces"
- Aditi Chattopadhyay**, Arizona State U., "Multidisciplinary Design Optimization Multiobjective Formulation Techniques"
- Weng Cho Chew**, UIUC, "Nonlinear Inverse Scattering of Large Objects using the Local Shape Function (LSF) Method" and "Multiple Scattering Study of Random Inhomogeneous Media using Supercomputers"
- Yee C. Chiew**, Rutgers U., "Force Biased Monte Carlo Simulation of Dense Chain Fluids"
- Shun Lien Chuang**, UIUC, "Linear and Nonlinear Optical Properties in Semiconductor Lasers and Optoelectronic Devices"
- Alexander Chudnovsky**, UIUC, "Numerical Simulation of Crack-Damage Interaction"
- Jacob Nan-Chu Chung**, Washington State U., "Direct Numerical Simulations of Laminar-Turbulent Transition in Mixed Convection Pipe Flow and Free Convection Boundary Layer Flow," "Direct Numerical Simulation of Flow Transition at Low Reynolds Numbers in a Vertical Pipe Flow," and "Heat Transfer Effects on the Structures of Transition in Blasius and Entrance Channel Flows: A Direct Simulation Study"
- T. J. Chung**, U. of Alabama, Huntsville, "Analysis of Turbulent Shock Wave Boundary Layers in Compressible Reacting Flows with Parallel Processing" and "Development of Parallel Computer Algorithm for Turbulent Compressible Reacting Flows"
- David Churchill**, Clemson U., "Fiber-Fiber Interactions in the Prediction of Elastic Properties of Short-Fiber Composites"
- M. E. Clark**, UIUC, "Cardiovascular System Simulation"
- Michael P. Cleary**, MIT, "Theoretical and Numerical Simulations of Hydraulic Fracturing Processes"
- Thomas F. Conry**, UIUC, "Thermal Analysis of Elastohydrodynamic Bearing Systems"
- Bruce A. Conway**, UIUC, "Direct Optimization of Dynamical Systems using Nonlinear Programming"
- Anoop K. Dhingra**, U. of Wisconsin, Milwaukee, "Complete Solutions to Polynomial Systems using Probability One Globally Convergent Homotopy Methods"
- Jeremiah F. Dwyer**, Montana State U., "Computational Analysis of Damage in Composites"
- Fangpu Gao**, UIUC, "Dimension Analysis on Finger Tremor in Tardive Dyskinesia Patients"
- Benjamin Gebhart**, U. of Pennsylvania, "Instability Analysis of Natural Convection along a Vertical Surface using Numerical Simulations"
- Ahmed F. Ghoniem**, MIT, "Numerical Simulation of Turbulent Combustion"
- Peyman Givi**, SUNY, Buffalo, "Direct Numerical Simulations and Large Eddy Simulations of Unpremixed Turbulent Reacting Flows"
- George Gogos**, Rutgers U., "Fuel Droplet Evaporation at High Pressure Environment; Natural Convection Effect"
- Stephen M. Goodnick**, Oregon State U., "NCE: Monte Carlo, Transport in Quantum Wires"
- Harold L. Grubin**, Scientific Research Assoc., "Computational Device Modeling"
- Robert B. Haber**, UIUC, "Supercomputer Applications in Design Optimization and Computational Solid Mechanics"
- George T. Hahn**, Vanderbilt U., "Analysis of Rolling Contact Deformation and Fracture"
- Thomas J. Hanratty**, UIUC, "Computer Experiments on Wall Turbulence"
- John G. Harris**, UIUC, "Scattering from Partially Closed Cracks and Other Imperfect Interfaces"
- James C. Hill**, Iowa State U., "Numerical Simulation of Nonreacting and Reacting Turbulent Flows"
- Antoine Kahn**, Princeton U., "Atomic Structure of Semiconductor Surfaces"
- Stephen F. Kawalko**, UIUC, "Electromagnetic Scattering by Impedance Bodies of Revolution with Fins"
- Ifiyenia Kececioglu**, UIUC, "Finite Element Computation of Multiphase Flow and Transport Problems"
- Jay M. Khodadadi**, Auburn U., "Numerical Simulation of Liquid Metal Flow and Heat Transfer in the Mold of Continuous Casters"
- Kyeykyoon Kevin Kim**, UIUC, "Exploratory Project" and "Stability of a Uniform Liquid Fuel Layer inside a Spherical-Shell Cryogenic Inertial Confinement Fusion Target"
- Doyle D. Knight**, Rutgers U., "A Compressible Navier-Stokes Algorithm using an Unstructured Adaptive Grid" and "3D Asymmetric Crossing Shock Wave-Turbulent Boundary Layer Interaction"
- Ranga Komanduri**, Oklahoma State U., "FEM Analysis of Various Manufacturing Processes"

Allocations continued on page 16

- Joel Koplik**, CUNY, "Molecular Dynamics of Fluid-Solid Systems"
- George Kosaly**, U. of Washington, "Investigation of the Laminar Flamelet Model of Turbulent Diffusion Flames"
- Ron D. Kriz**, Virginia Polytechnic Inst. & State U., "Simulation and Visualization of Stress Wave Propagation near Fiber-Matrix Interphases: Scanning Acoustic Microscope Simulation for Determining Interphase Structure"
- Anil K. Kulkarni**, Pennsylvania State U., "Flow Characteristics of a Precessing Deflected Jet"
- Richard T. Lahey, Jr.**, Rensselaer Polytechnic Inst., "The Development of Multidimensional CFD Capabilities for Multiphase Flows"
- Douglas A. Lauffenburger**, UIUC, "Monte Carlo Simulations of Cell Shape and Adhesion"
- Shung-Wu Lee**, UIUC, "Computation and Visualization of Electromagnetic Scattering"
- Wilbert Lick**, U. of California, Santa Barbara, "Sediment and Contaminant Transport in Aquatic Systems"
- Gang Lin**, Louisiana Tech U., "Design Optimization of Herring Bone Air Bearings"
- J. Bruce Litchfield**, UIUC, "Measurement of Transient Moisture Profiles and Structural Changes Using 3D NMR Microscopy"
- Wing Kam Liu**, Northwestern U., "Computer Modeling of Material Forming Processes with Micro/Macro Crack Damage Accumulation"
- Eric Loth**, UIUC, "Bubble Dispersion and Modulation," "Shock Interaction with Rigid Bodies and Mixing Layers," and "3D Shock Interaction with Rigid Bodies and Mixing Layers"
- Joseph W. Lyding**, UIUC, "The Distributed Scanning Tunneling Microscopy Laboratory"
- Karthikeyan Mahadevan**, UIUC, "Development of New Finite Element Algorithms for the Solution of 2D and 3D Electromagnetic Scattering Problems"
- Paul E. Mayes**, UIUC, "Electromagnetic Radiation and Scattering from Conducting Surfaces in Free Space"
- Raj Mittra**, UIUC, "Time Domain Electromagnetic Analysis of Interconnects in Digital Computer Systems"
- Satish Nair**, U. of Missouri, Columbia, "Computations for Dynamic Systems with Neural Network and Fuzzy Logic Control Algorithms"
- Raghu N. Natarajan**, Rush-Presbyterian St. Luke's Med. Center, "Mechanical-Biological Interaction with Treatment of Joint Diseases"
- Andrew R. Neureuther**, U. of California, Berkeley, "TEMPEST"
- Ahmed K. Noor**, U. of Virginia, "Nonlinear Finite Element Dynamic and Postbuckling Analyses on Multiprocessor Computers"
- Lorraine Olson**, U. of Nebraska, Lincoln, "Improved Model Techniques for the Inverse Problem of Electrocardiography"
- Kook D. Pae**, Rutgers U., "Computational Modeling of Hydrostatic Metal Forming Processes"
- Mangalore A. Pai**, UIUC, "High-Speed Simulation of Large-Scale Dynamic Power System Models"
- Stanley L. Paul**, UIUC, "Validation of Structural Analysis Techniques using Field Test Data"
- Dimos Poulikakos**, UIUC, "Numerical Simulation of Splat Quench Solidification"
- Umberto Ravaioli**, UIUC, "Study of Transport in Deep Sub-micron MOSFETS using a Full Bandstructure Monte Carlo Approach," "NCEE: Monte Carlo, Mode Matching," "Code Performance Analysis," "Special Projects (CRAY Y-MP)," "Special Projects (CRAY-2)," and "Molecular Dynamic Algorithms for Monte Carlo Simulation of Semiconductor Transport"
- Chittaranjan Ray**, Ill. State Water Survey, "Modeling Transport of Agricultural Chemicals in a Dual-Porosity System Resulting from Macropores"
- Jorge Rodriguez**, Rutgers U., "Nonlinear Analysis of WMBAR Motion Segments"
- Vythilingam Sathiaselalan**, Northwestern U., "Computer Simulation Studies for Electromagnetic Hyperthermia"
- William Raymond Schowalter**, UIUC, "Die Swell of Emulsions"
- Justin Schwartz**, UIUC, "Mechanical and Magnetothermal Optimization of Superconducting Magnets for Large-Scale Applications"
- Huseyin Sehitoglu**, UIUC, "Modeling of Microstructure Effects on Fatigue Crack Closure"
- James A. Sherwood**, U. of New Hampshire, "Investigation of the Thermomechanical Response of a Titanium Aluminide/Silicon Carbide Composite using a Uniform State Variable Model and the Finite Element Method"
- Wei Shyy**, U. of Florida, "Numerical Prediction of Transport Characteristics and Macroseggregation of Superalloy Processing"
- Alfredo Soldati**, U. of California, Santa Barbara, "Direct Simulation of the Electrohydrodynamic of Electrostatic Precipitators"
- Mark Allen Stadther**, UIUC, "Strategies for Using Advanced Computer Architectures in Designing Complex Chemical Process"
- Scott D. Stewart**, UIUC, "Numerical Simulations of Detonation Dynamics"
- Gregory E. Stillman**, UIUC, "Quantum Well Detectors"
- Larry Taber**, U. of Rochester, "Theoretical Models for the Embryonic and Mature Heart"
- Christos George Takoudis**, Purdue U., "Thin Film Deposition of Patterned Substrates from Silicon Tetrachloride-Based Systems: Relationships between Material Properties and Processing"
- Troy Torbeck**, UIUC, "Startup-Postive Crank Case Ventilation Studies"
- George S. Triantafyllou**, CUNY, "3D Interaction of a Vorticity Field with the Ocean Surface"
- Keh C. Tsao**, U. of Wisconsin, Milwaukee, "Combustion System Design of High-Output Diesel Engine"
- Surya Pratap Vanka**, UIUC, "Direct and Large-Eddy Simulations on Massively Parallel Computers" and "Higher Level Simulations of Complex Fluid Flows"
- Frank B. Van Swol**, UIUC, "Micelle Formation at the Fluid-Wall Interface" and "Molecular Dynamics Studies of Micellar Solutions"
- Jonathon C. Veihl**, UIUC, "Antenna Analysis in Complex Environments"
- John Scott Walker**, UIUC, "High-Velocity Boundary and Interior Layers in Liquid-Metal Magnetohydrodynamic Flows"
- William M. Worek**, UIUC, "Heat Transfer and Fluid Flow in Planar 90 Degree Bifurcations with and without Rounded Corners"
- Hu Yang**, U. of Akron, "Parallel Finite Elements Method on MIMD and SIMD Systems"
- Yook-Kong Yong**, Rutgers U., "Numerical Analysis of Very High Frequency, Piezoelectric Quartz Crystal Resonators"

For details about how to apply for time on NCSA's high-performance computing systems, contact MetaCenter Allocations (see [neca contacts](#), page 2). ▲

CM-5 enhancements attract friendly users

by Michael Welge, Research Programmer, Computational Mathematics and Computer Science Team

A year ago the first CM-5 hardware shipping crates arrived at NCSA [see *access*, May-June 1992]. Since that time, the CM-5 friendly user community has experienced several hardware changes that have greatly enhanced the viability of the system for Grand Challenge scientific computations.

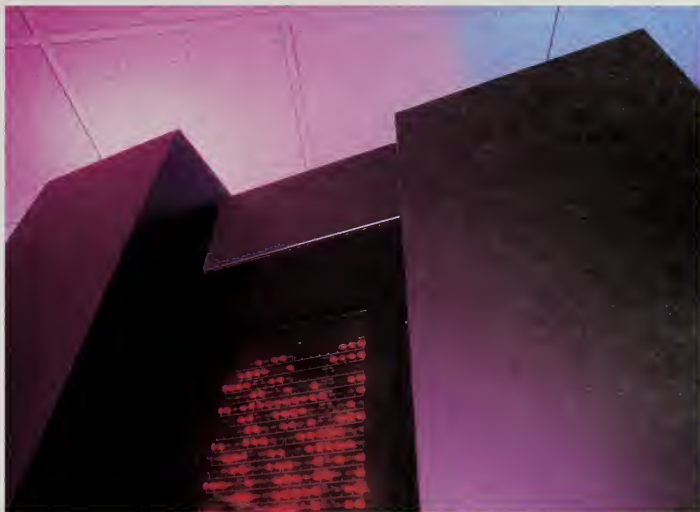
The CM-5, Connection Machine (Model 5), is designed by Thinking Machines Corp. (TMC), Cambridge, MA.

Hardware enhancements

NCSA's CM-5 initially supported 512 RISC processors. This basic processing node consisted of a microprocessor, memory subsystem, and a CM-5 network interface all connected to a standard 64-bit bus. The SPARC microprocessor, running at 32 MHz, is capable of 22 MIPS and 5 Mflops.

Today, NCSA's CM-5 has been optionally configured with the Datapath floating point system (also referred to as DASH, or vector units). There are four vector units per node, all running under control of the SPARC microprocessor. One memory and two arithmetic operations (mult, add) can be performed per vector unit per clock cycle. The vector unit clock rate is 16 MHz, and peak performance is 128 Mflops per node. This upgrade increased the aggregate theoretical performance from 2.5 to 64 Gflops and the DRAM memory from 8 to 16 Gbytes.

The addition of the 100 Gbyte Scalable Disk Array (SDA) in mid-April provides an extremely high-performance, highly expandable disk storage system comprised of Disk Storage Nodes. The basic Disk Storage Node—which provides 9.2 Gbytes of storage, a peak bandwidth over 17 Mbytes per second, and 25 MIPS of processing power—comprises a controller built on a SPARC processor, a network interface, a large disk buffer, four advanced SCSI controllers, and eight 3.5" hard disk drives. These SDA Disk Storage Nodes—analogous to the computational processing nodes—are directly connected to the CM-5 internal network.



This direct connection enables each Disk Storage Node to contribute not only to storage capacity but also to I/O performance. The number of Disk Storage Nodes in the SDA can be increased or decreased, thereby achieving an I/O system matched to the performance and capacity needed for the user's application. NCSA's CM-5 SDA consists of 12 Disk Storage Nodes that provide 100 Gbytes of storage at I/O bandwidths of up to 132 Mbytes per second sustained.

CM-HIPPI arrives soon

NCSA's user community will experience increased transfer rates from the CM-5 to other supercomputer systems when the CM-HIPPI device is ready later this year. CM-HIPPI is an integrated system that receives CMFS files system commands from the CM-5 control processor. The CM-HIPPI contains a CPU, disk drives, a VME bus, and HIPPI I/O interface modules. The CM-HIPPI connects directly to the CM-5 network to provide 1 gigabit aggregate bandwidth.

In mid-September a TMC CM-5 testbed system with a HIPPI interface was installed at NCSA. Its goal is to

NCSA's CM-5. (Photo by Wilmer Zehr)

support UIC/NCSA's CAVE (Cave Automatic Virtual Environment) demo at Supercomputing '93. It will also allow for a smooth integration of HIPPI into NCSA's CM-5 production system.

CM-HIPPI team members are Randy Butler, group leader; Joseph Godsil; Vijay Rangarajan; Von Welch; and Paul Zawada.

Applications research efforts

Many users took advantage of the CM-5 friendly user period to make use of the increased performance of the distributed memory CM-5. Many of those same users continue computing on the CM-5, which entered into production in May.

CM-5 users and their areas of research are listed on the following page. Watch for reports of some of their research in the next issue of *access*, which will focus on Grand Challenge research.

Astronomy and gravitation

Richard Crutcher
Astronomy
UIUC

David Wesley Hobill
Physics/Astronomy
Univ. of Calgary

Computational biology

Roscoe Giles
Electrical, Computer, and Systems
Boston Univ.

Michael Keegan
Institute for Computational Science
George Mason Univ.

Ronald Levy
Chemistry
Rutgers Univ.

James Andrew McCammon
Chemistry
Univ. of Houston, University Park

Klaus J. Schulten
Physics
UIUC

Earth, environmental, and social sciences

Richard K. Sato
Scientific Computing Division
NCAR

Fred Sklar
Southern Florida Water Survey

Engineering sciences

Weng Cho Chew
Electrical/Computer Engineering
UIUC

Sanjay Mehrotra
Industrial Engineering/Management
Sciences
Northwestern Univ.

Dennis Parson
Civil Engineering
UIUC

Otmar S. Schlunk
Electrical/Computer Engineering
UIUC

Kim Simmons
Nuclear Engineering/Engineering
Physics
Univ. of Wisconsin, Madison

Surya Pratap Vanka
Mechanical/Industrial Engineering
UIUC

Mathematics and computer science

Andrew Chien
Computer Science
UIUC

George Cybenko
Thayer School of Engineering
Dartmouth College

Dennis Gannon
Computer Science
Indiana Univ.

Ewing Lusk
Mathematics/Computer Science
Argonne National Laboratory

David Padua
CSRD
UIUC

Quantum systems

Ronald E. Cohen
Geophysical Laboratory and Center
for High Pressure Research
Carnegie Mellon Univ.

Arthur Freeman
Physics/Astronomy
Northwestern Univ.

Rajan Gupta
Los Alamos National Laboratory

Herbert W. Hamber
Physics
Univ. of California, Irvine

John B. Kogut
Physics
UIUC

Don Secrest
Chemistry
UIUC

Robert Sugar
Physics
Univ. of California, Santa Barbara

Industrial users

Ramesh K. Agarwal
McDonnell Douglas Research
Laboratories
McDonnell Douglas Corp.

Caterpillar
FMC
Lilly
J. P. Morgan
United Technologies Research Center

NCSA users

Fouad Ahmad—Engineering sciences
David Ceperley—Quantum systems
Michael Heath—Mathematics and
computer science
Eric Jakobsson—Molecular dynamics
Michael Norman—Astrophysics
Clint Potter—Biomedical imaging
Ed Seidel—Gravitation
Danesh Tafti—Computational fluid
dynamics
Robert Wilhelmson—Earth sciences

Contact MetaCenter Allocations
for details about how to apply for
time on NCSA's high-performance
computing systems [see **ncsa**
contacts, page 2]. ▲

sized companies simply do not own or have access to Cray computers—they typically do all of their engine development using simplified, zero-dimensional tools on PCs or workstations. The answer, according to Assanis, is parallelization of KIVA—a task that KIVA's developers at LANL are currently pursuing. NCSA is working with LANL and Thinking Machines Corp. to port KIVA to NCSA's CM-5. Assanis will then incorporate his latest models of engine flow and spray processes into the parallelized version of KIVA.

Not only would parallelization allow the modelers to introduce even more variables into their calculations and achieve finer grid resolution, but a parallelized code would be faster and could be ported to clusters of networked workstations.

Solving flows in two-stroke engines

Assanis and his students have developed a code, ARIS-3D, designed to study 3D flows in complex geometries. Intake and exhaust occur simultaneously in two-stroke engines,

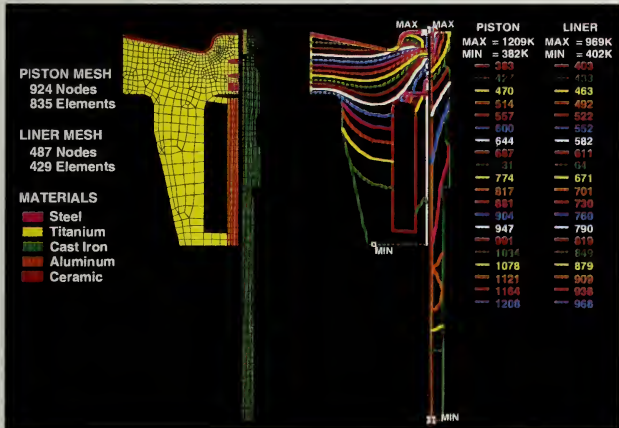
which are currently used to power motorcycles, snowmobiles, and lawn mowers. In a single revolution, a fresh fuel mixture must enter the combustion chamber while displacing the exhaust mixture—a process known as scavenging. "Unless you are very careful," says Assanis, "you can have many recirculation zones in the chamber full of unburnt fuel and exhaust products." This results in reduced fuel efficiency and increased hydrocarbon emissions.

Two-stroke engines may be the automobile engine design of the future, according to Assanis, if the scavenging process can be improved so that the engines can meet emission standards.

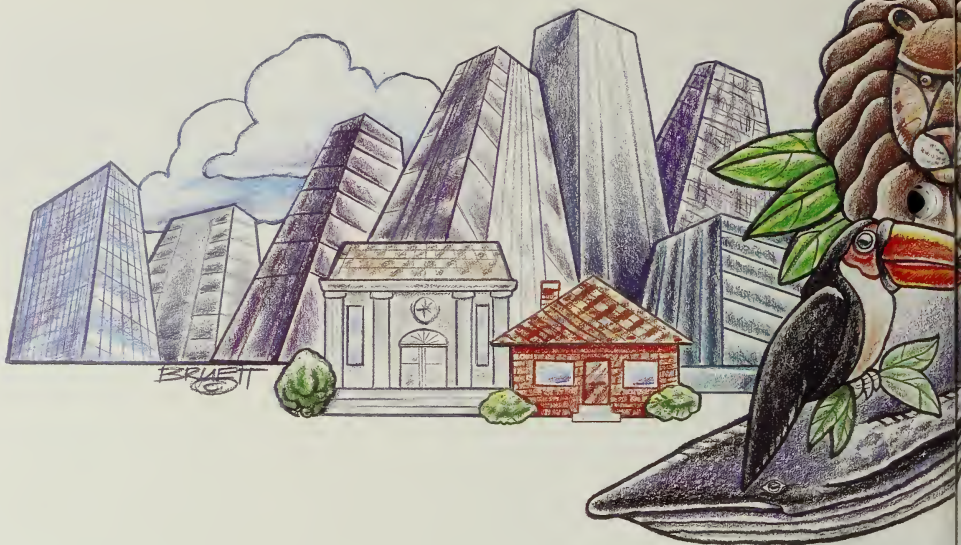
"If a code is ever to be successful," says Assanis, "you need the participation and close collaboration of the modeler; the experimentalists who validate the models; the specialists in visualization, parallelization, and algorithm development; and from designers in industry. We will see a lot more multimachine, multiperson collaborations in the future." ▲



Dennis Assanis (photo by Thompson-McClellan Photography)



Finite element analysis of transient heat flow through a low-heat rejection piston-liner design. (Left) Component meshes illustrating design with various insulating materials. (Right) Temperature contours at top dead center predicted using gas-side boundary conditions from KIVA. (Courtesy David Baker and Dennis Assanis)



ENVISIONING THE EARTH: THE GEOSPHERE PROJECT

BY SARA LATTA, SCIENCE WRITER

The late Nobel Prize-winning physicist Richard Feynman called Tom Van Sant "the only truly modern artist that I know," citing Van Sant's appreciation of technology and science and his incorporation of them into his work. Yet, there is something fundamental about Van Sant's vision: "We spent a couple of million of years evolving as a species . . . understanding our world through visualization," Van Sant said at an NCSA lecture at the Beckman Institute in March.

"A few hundred years ago, modern cultures committed themselves to the written word as a way of storing and disseminating information," he continued. "While this was obviously beneficial . . . it also committed us to linear thinking. We soon realized that we could not handle [the information] unless we started chopping it up into segments and compartmentalizing it into a library. But nature is not compartmentalized: it is a symbiotic continuum."

The Geosphere Project, founded in 1989 by Van Sant—also its CEO—is based on the painter-sculptor-architectural designer's dream that complex Earth resource management

and global change issues could—and should—be understood as a symbiotic continuum by policy makers, the research community, educators, and the lay public alike. As an artist, he realized that the only way to understand the complex relationships between the many Earth resource management issues was through visualization.

*" . . . Nature is not
compartmentalized;
it is a symbiotic
continuum."*

—Tom Van Sant

Reality models of the Earth

The first product of the Geosphere Project was a global map, at 4 kilometer resolution, made by digitally piecing together thousands of cloud-free satellite photos of the Earth,

gleaned from National Oceanic and Atmospheric Administration (NOAA) archives. The map, which took 10 months to complete, depicts both hemispheres of the Earth in the summer. It is color converted so that oceans appear blue; forests, green; and deserts, brown—as we would see it from space. A 1k resolution image of the Earth and a series of geosphere globes are in the works, onto which a variety of databases can be projected.

Plans are underway to use the globe data in the CAVE (Cave Automatic Virtual Environment)—a virtual reality, or VR, laboratory designed to surround the viewer with data at UIC's Electronic Visualization Laboratory (EVL). NCSA will soon have access to the globe data in an interactive environment as well, when EVL completes construction of a CAVE at NCSA's VR Laboratory.

With the CAVE technology, a viewer could stand inside the globe, as it were, viewing the globe from the inside out. This perspective would give the viewer a much larger distortion-free perspective of the globe.

Geosphere continued on page 22



(Illustration by Carlton Bruett)

INTEGRATING GLOBAL MODELS: CONFERENCE REPORT

BY RANDALL GRAHAM, SCIENCE WRITER, AND FRAN BOND, PUBLICATIONS EDITOR

"Ecological economics is an attempt to integrate social sciences and natural sciences in order to provide the information necessary to formulate policy dealing with global climate change," said Karl-Göran Maler, director of the Beijer International Institute for Ecological Economics, a research institute of the Royal Academy of Sciences, Stockholm, Sweden. "In order to do that, we have to construct an understanding of the processes which join the social systems to the natural systems."

Maler spoke to about 30 scientists (see list on page 22) who gathered for the Global Ecological Economic Modeling Conference in March at the Beckman Institute. NCSA co-sponsored the conference with the Beijer Institute. Robert Costanza, president of the International Society for Ecological Economics and a research affiliate of the Beijer Institute, coordinated the conference.

The conference focused on constructing a new global model of the Earth by joining techniques from social science and natural science. It is widely thought that such a model

could clarify humankind's impact on Earth's ecosystems and climate [see *access*, July–September 1992].

Attendees gathered to form research alliances for the future and to collaborate on a preproposal for funding global modeling R&D. After a day of presentations that introduced each other's research and modeling processes, conferees divided into small working groups to discuss and hone issues that were then formulated into a formal document.

Ecology

"Our goal is to build an evolutionary, adaptive modeling environment rather than a specific model," explained Costanza, professor of ecology at the University of Maryland and director of the Maryland International Institute for Ecological Economics. "We want the model to continue to progress." He said that the model could be used in conflict resolution.

The conferees were seeking a new modular approach to model building that could evolve over time through adaptations and improvements. According to Costanza, they did not

want to "build it once, get the answer, and quit." This was to be the first step in an ongoing endeavor.

Ecological economics

NYU's Ecological Economist Faye Duchin said the timing could not have been better for linking the model she uses with those of others. "We have done a lot of theoretical work in the last decade that has not been brought in [to the model], and we were ready to rewrite the model to make it more transparent to others."

She and her colleagues use a model developed by the Nobelist Wassily Leontief. Duchin directs the Institute for Economic Analysis founded by Leontief.

Duchin felt the conference broke new ground: "At a conceptual level none of us are yet asking the most strategic global questions because each of us is only asking the questions that appear to be globally strategic in our own area."

Global models continued on page 23



"We spent a couple of million years evolving as a species . . . understanding our world through visualization," says Tom Van Sant, founder and CEO of the Geosphere Project.

(Photo by Thompson-McClellan Photography)

Geosphere continued from page 20

NCSA is also exploring the possibility of allocating supercomputer time for the production of the 1k geosphere image, according to NCSA Director Larry Smarr.

"Now we can look at a reality model," said Van Sant. "That's very important for us. Political boundaries cannot be seen from space. They are an artificial concept that we superimpose, I'm sure for many good reasons, but not necessarily for reasons of Earth resource management."

The Geosphere Interactive Visual Library

Van Sant is gathering and creating visualizations for global databases acquired from NOAA, the National Aeronautics and Space Administration, The World Bank, the National Geographic Society, the World Conservation Monitoring Centre, and other government and nongovernment organizations. The databases are digitized, coregistered in geographic information systems, rendered for overlays, and animated for time-lapse sequences and zooms. Integrated databases can provide for layered viewing, special effects, or

flight simulations. The product is a laser disk prototype of the Geosphere Interactive Visual Library, which debuted with great success at the Earth Summit in Rio de Janeiro, June 1992.

The library's interface is a map of the Earth with various icons representing geographic, human, land, and animal systems. The viewer might select the habitat of the Asian elephant, from the 1970s to the present time, for example. By overlaying this database with agricultural, demographic, and other databases, the viewer can easily understand the relationships between the activities of elephants and man. Or, by selecting an icon representing the South American rainforests, overlaid databases can show that slash and burn deforestation is related not only to the reduction of species habitat, but also the depletion of the already scanty topsoil, the pollution of the streams and ocean reefs, the release of CO₂ into the atmosphere, and large releases in methane—the result of an increase in the termite population.

Van Sant envisions a library on each continent someday—housed in what he calls an "Earth Situation Room," the post-Cold War version of the War Room. The library would be networked so that anyone with a computer terminal could access the information.

Kids doing real science

Van Sant believes that "kids can do real science, particularly if they can interactively overlay databases."

For example, Van Sant has a database from the U.S. Naval Postgraduate School in Monterey, CA that shows all of the surface currents off the California coast. He also has a database of the migration pattern for gray whales from the Bering Strait to Baja California, where they calve and breed. Do the whales swim against or with the current? It is probably of some interest, but no one has bothered to overlay the two databases.

"I'm saving these kinds of problems for the kids in the pilot programs," Van Sant said. "We can start empowering kids to not only do the work, but then perhaps even stand up and join in policy, to claim their inheritance; the resources that are being used in a unsustainable manner."

"We are in the system"

"I think people are responding more to the Earth, and to Earth resource management, because we just finished exploring the solar system," said Van Sant. "We found out that there is a very narrow hospitality zone for life."

"Bucky Fuller said that we are passengers on the spaceship Earth. Well, we are really not passengers on anything. We are more like part of the upholstery, so to speak. It is us, and we are it, and we are in the system." ▲

Global Ecological Economic Modeling Conference Attendees

Lars Bergman, Stockholm, Sweden
Robert Costanza, U. of Maryland
Ralph d'Arge, U. of Wyoming
Kieran Donaghy, UIUC
Faye Duchin, NYU
Charles Falkenburg, U. of Maryland
Bruce Hannon, UIUC
Robert Herendeen, INHS
John Hobbie, Marine Biology Lab,
Woods Hole
Robert Kaufmann, Boston U.
Eric Lambert, CERL
Glenmarie Lang, NYU
Robert Lempert, RAND Corp.
Robert Lutz, CERL
Karl-Göran Mäler, Beijer Institute
Tom Maxwell, U. of Maryland
Gottfried Mayer-Kress, UIUC
Helena Mitasova, CERL
Matthias Ruth, Boston U.
Michael Schlesinger, UIUC
Mark Schwartz, INHS
Kevin Seel, CERL
Steve Seitz, UIUC
Jason Shogren, Yale U.
Fred Sklar, Florida Water
Management
Michael Sonis
James Westervelt, CERL

Climate

Climatologists' models are complex because they render a number of variables in 3D. According to UIUC Professor of Atmospheric Sciences Michael Schlesinger, "The whole spectrum of human endeavors, including agriculture and the ability to maintain water quality, is influenced by climate. We do not have a good understanding of how this works, because we need information on the small scale at which impacts are felt. . . . We are also held back by our understanding of how the processes work in the climate system. The problem, as I see it, is to ask 'Well so what if climate changes?'"

Geography

UIUC Geography Professor Bruce Hannon was NCSA's host and co-coordinator for the conference. Together with an international group of scientists, including Costanza, Hannon visited the Beijer Institute in the summer of 1992 (see photo below right). He returned in September 1993 for the 4th Annual International Complex Systems Conference. NCSA Director Larry Smarr attended also.

We are in "the infant stage of the modeling process," Hannon acknowledged. "Both data and the modeling process need to be addressed. . . . Although many of the ecological modelers are using STELLA, there was talk of needing [more complex] software to integrate the federation that goes into producing a large global model. NCSA has a software development initiative to address this."

As a participant in this initiative, Hannon is a visiting professor at NCSA, where he has been enhancing modeling techniques and running code on the CM-5 [see *access*, October–December 1992]. Albert Cheng, NCSA Software Development Group (SDG) programmer, is working with Hannon on this effort, which was demonstrated. Duchin showed a software program she developed with SDG Programmer Jason Ng.

Goals of the group

"We are interested in how to make connections between various models and also in how that coupling affects our model," said Hannon, summarizing the conference's goals. "For us it means moving from 30 x 60 meter cells to much larger ones for the global model."

Costanza joined in: "People at the conference are working on stand-alone parts of the global model. . . . What we want to view is the whole. This is conceived of as a 5-year project," he continued. "The model structure itself will be evolving."

The group dealt with seemingly astounding datasets in terms of variables, but their vision is equally challenging. Since the "endgame" of their efforts could have broad, worthwhile consequences, the group gathered at the conference were dedicated to the long term.

According to Duchin, this ingathering of researchers showed that "science can be used to solve real world problems. . . . The issue here," she said, "is that the way we are living on this planet is causing repercussions that are bound to feed back on us. . . . Our conviction is that [humankind is] probably going to have to make more significant changes in how we live than most people have allowed their imaginations to consider." ▲

"[We are in] the infant stage of the modeling process."

—Bruce Hannon



(Top) Attendees at the Global Ecological Economic Modeling Conference included (left to right) Karl-Göran Maler, director of the Beijer Institute; Robert Costanza, director of the International Society for Ecological Economics; Michael Schlesinger, UIUC professor of atmospheric sciences; Larry Smarr, director of NCSA; Faye Duchin, director of the Institute for Economic Analysis; and Bruce Hannon, UIUC professor of geography on sabbatical to NCSA. (Photo by Thompson-McClellan Photography)

(Bottom) Pictured at the Beijer Institute in Stockholm are (left to right) Carl-Olof Jacobson, general secretary of the Royal Swedish Academy; Costanza; Joseph Hardin, NCSA associate director for the Software Development Group; Maler; and Hannon. (Photo by Lars Falck, courtesy of Bruce Hannon)

CATERPILLAR WINS GRAND CHALLENGE AWARD

BY CATERPILLAR INC.



"With virtual reality," says Caterpillar Design Engineer Dave Stevenson, "we can evaluate dozens of design options." Wearing a Virtual Research Flight Helmet, Stevenson simulates "driving" a Caterpillar machine on Silicon Graphics' Skywriter workstation. (Courtesy Caterpillar Inc.)

Caterpillar Inc. received NCSA's top corporate honor for its use of virtual reality and HPCC to design some of its best-selling machines. The Grand Challenge Award—to recognize breakthrough research resulting from an NCSA partnership—was presented to Caterpillar at the Fifth Annual Executive Meeting of NCSA's Industrial Partners in May 1993.

"Caterpillar's research work on this project is very significant because of the improvement to their design process," says John Stevenson, NCSA's corporate officer and head of the Industrial Program. "This will help improve the company's ability to compete globally."

Designing with virtual reality

Caterpillar received the award for effectively using virtual reality and HPCC technology to improve visibility for drivers in the cabs of its wheel loaders and backhoe loaders. These machines are used to build roads, dig foundations, load trucks, and haul loose materials such as gravel. A cab's visibility affects an operator's productivity, comfort, and safety.

Through virtual reality, engineering blueprints become 3D, allowing engineers to see how their designs will work in a seemingly real world. Hundreds of thousands of mathematical computations are almost instantaneously translated into a simulated environment that the operator can "see" by wearing a special helmet (see photo left).

This year's award recognizes the efforts of design engineers Dave Stevenson of the Wheel Loader and Excavator Business Unit, Aurora, IL, and John Bettner of the Building Construction Products Division, Clayton, NC.

"This technology allows us to dramatically shorten the amount of time it takes to analyze a new design concept and incorporate it into our production process," says Dave Stevenson. "It also represents a sizable cost savings because we are not having to build prototype machines or make last-minute design changes." Design engineer Stevenson says that when Caterpillar researchers relied on conventional design methods, they spent from six to nine months building full-scale models and evaluating design changes. With virtual reality, multiple design options often can be evaluated in less than a month.

A number of design options already have been tested for new models of Caterpillar wheel loaders and backhoe loaders that will be introduced by 1996. The company also plans to eventually allow customers to "field test" new product designs using virtual reality technology.

Caterpillar/NCSA partnership
Caterpillar, headquartered in Peoria, IL, is the world's largest manufacturer of earthmoving and construction equipment and a major manufacturer of diesel and natural gas engines. The corporation joined NCSA in August 1989 through a multiyear, multimillion-dollar agreement. Caterpillar engineers working in Champaign and from Peoria, via remote linkage to NCSA's supercomputers, receive access, training, and extensive experience with the latest computing capabilities.

AT&T, Dow Chemical Co., Eastman Kodak Co., Eli Lilly & Co., FMC, J. P. Morgan, Motorola Inc., Phillips Petroleum Co., Schlumberger, and United Technologies Corp. are NCSA's other partners.

NCSA established the annual Industrial Grand Challenge Award last year [see *access*, May-June 1992] to recognize corporations who accomplish breakthrough research through their NCSA partnership to improve product development and quality. ▲

EDITOR'S NOTE: Caterpillar's award and use of virtual reality was featured in 45 media outlets, including:

- Associated Press
- CNN
- Chicago Sun-Times
- Cleveland Plain-Dealer
- Houston Chronicle
- HPCWire
- National Public Radio
- United Press International
- The Wall Street Journal
- Washington Times



Dave Stevenson (left) and John Bettner (right) display their Industrial Grand Challenge Awards presented by NCSA Director Larry Smarr (center). Images of the abacus and CM-5 in the background of the plaques symbolize the growth in computing; pictures of Caterpillar vehicles in the foreground represent the researchers' work. (Photo by Wilmer Zehr)



Partner executives and NCSA staff met for the Fifth Annual Executive Meeting of NCSA's Industrial Partners to discuss new high-performance computing technologies and strategic business importance. (Photo by Wilmer Zehr)

MODELING DISPOSABLE DIAPERS

BY LEE M. HUBER, ONSITE REPRESENTATIVE, THE DOW CHEMICAL COMPANY



Still image from animation showing simulation of fluid diffusion through a heterogeneous medium—cellulose fluff with embedded SuperAbsorbent Particles (SAP). (Courtesy Lee Huber, Dow Chemical Co., research; Michael McNeill, visualization)

A Dow Chemical Company project, carried out by Dow's Kishore Kar, is producing a diaper design incorporating Drytech® superabsorbent polymer particles distributed in a fluff pad. The design was evaluated using a computer model run on NCSA's CRAY-2 system.

NCSA research programmer Michael McNeill visualized the results by using a high-performance Silicon Graphics Inc. workstation. A still from the visualization [left] shows the computational grid that extends over a quarter of the diaper. Polymer particles are represented by spheres. The concentration of liquid and its motion, described as a function of time, are represented by the variation in color from violet to brown as well as the isometric surfaces. Numerical results, which were obtained at many

timesteps, were converted to images and animated to view the time evolution of the process. The overall model was compared to a magnetic resonance imaging experiment, which provides a three-dimensional image of the water distribution in a diaper, and was shown to give comparable results to the final steady-state values.

This new way of visualizing diaper performance with HPCC techniques is facilitating the development process for improved disposable diapers.

More information about this project and other HPCC MetaCenter research efforts is available on the NCSA World Wide Web server at the following URL: http://www.ncsa.uiuc.edu/Pubs/MetaCenter/SciHi93/O.Highlights_Contents.html ▲

* Drytech is a trademark of the Dow Chemical Company.

AT&T's XUNET DEMONSTRATED FOR GORE

Early in May Vice President Albert Gore toured AT&T Bell Laboratories at Murray Hill, NJ and saw a demonstration of the XUNET/BLANCA project with NJ Governor Jim Florio and U.S. Senator Frank Lautenberg.

Afterwards AT&T announced that a major step forward had been taken in making the vision of a national information superhighway a reality. Now operating the nation's fastest wide-area Asynchronous Transfer Mode (ATM) network over fully optical links, the experimental research network will help in the development of commercial ATM networks. AT&T's 500-mile fiber optic network runs at 622 Mbps (megabits per second). The new network is an enhancement to AT&T's existing Experimental University Network (XUNET), an ATM network that connects seven leading research laboratories and universities and three AT&T switching sites nationwide.

The new 622 Mbps links will remain connected to the rest of the XUNET, which uses ATM at 45 Mbps, through AT&T's XUNET experimental switch in Chicago. XUNET, sponsored by the Corporation for National Research Initiatives (CNRI) with funding for research provided by NSF and ARPA, forms an integral part of the BLANCA Gigabit Testbed [see *access*, September–October 1990]. The network currently links the University of Wisconsin at Madison, the University of Illinois at Urbana-Champaign, the University of California at Berkeley, Rutgers University, AT&T Bell Laboratories, Sandia

National Laboratory, Lawrence Livermore National Laboratory, and three AT&T network switching sites.

With the speed of this network, the entire contents of the Encyclopedia Britannica—approximately 13 million words—could be transmitted in less than 1 second. (The same amount of information sent from a home PC via the usual modem speed would take more than 2 1/2 days.)

Networks such as XUNET could revolutionize people's lives. For example, high-resolution images of complex medical data, such as x-rays and scans, could be transmitted nearly instantaneously from a remote hospital to a specialist located across the country or the world to save diagnostic time. Designers would be able to use their desktop workstations to harness the power of remote supercomputers to build 3D prototypes of products. Interactive multimedia audio, full-motion video, and imaging conferences could bring people from distances together as if they were physically in the same room.

The fully optical network from Madison, WI to Champaign-Urbana, IL is connected through the AT&T XUNET testbed ATM switch in Chicago and uses optical amplifiers which carry much higher speed signals than previously. The network has undergone operational testing and is currently active. Work will continue in the areas of HPCC applications testing, including real-time networking, multimedia, and desktop videoconferencing. ▲

ISDN links C-U schools to NCSA

by Sarah Thomas, Graduate Student, UIUC School of Library and Information Science

NCSA's Education Group is training and encouraging local elementary and high school teachers to use computers (including supercomputers) in their teaching. Through the ISDN (Integrated Services Digital Network) connection project, teachers and students can experiment with HPCC and obtain results in their classrooms in seconds or minutes. Using a micro-computer alone would take hours or days.

Eight schools in the Champaign-Urbana area were selected to receive ISDN lines connected to the campus network at UIUC: Leal Elementary, Urbana Middle, and Urbana High (Urbana); Centennial High, Central High, Franklin Middle, Dr. Howard Elementary, and Holy Cross (Champaign).

Ameritech donated the equipment necessary to install the ISDN lines, with the agreement that a six-month trial would be run to assess the benefits of the connection and to examine the possibilities for enhanced education through the use of computers by teachers and students.

Enabling "real science"

An objective of the Education Group is to encourage teachers and students to do "real science in real classrooms on real computers." Robert Panoff, senior research scientist at NCSA, clarifies this concept by explaining that most science education software only allows students to work with watered-down simulations or animations, which often distort real conditions and obscure the true nature of the objects being studied.

By having access to data from realistic simulations—which often require the power of a supercomputer to run—and from direct observations, such as satellites or online telescopes, students gain a more accurate view of what real science is.

Providing software

For example, the link with the campus network enables teachers and students to access data often discussed in science and math classes, such as the UIUC weather station. Satellite images that are updated every hour can be viewed in the classroom. In addition to weather data, the ISDN connection enables teachers and students to experiment with interactive computing on a supercomputer. ▲

How ISDN circuits work

A generic model of an ISDN line consists of two 64 kb/s circuit-switched channels (called B- [Basic] channels), and one 16 kb/s packet-switched channel (the D- [Data] channel). The B-channels carry data transmitted by the user, while the D-channel carries control information for the B-channels from the network to the user. The D-channel can also carry a limited amount of packet-switched data, but for the most part, this is the function of the B-channels.

Most of the local ISDN upgrade was done at the telephone switching station. Elementary schools were given one B-channel; high schools got two. At the end of the ISDN line to the schools are IMACs. These are linked by Ethernet cable to Gatorboxes. Each school has a separate Gatorbox to reduce traffic. TCP/IP local talk network runs on the lines, but any protocol can be used. AppleTalk cables connect up to 15 personal computers to the Gatorbox. Each computer has an IP address; up to 15 addresses can be administered through the IMAC.

Real Science
in
Real Classrooms
on
REAL
Computers!

Software

for math & science

by Sarah Thomas, Graduate Student, UIUC School of Library and Information Science

NCSA is developing software and experimenting with commercially available software programs for teaching math and science. Teachers are encouraged to participate in programming efforts and software design that address concepts they are teaching.

Development of Fractal Microscope software

One of the software programs being used at this time is Fractal Microscope, which was developed by Panoff and Michael South, an REU intern at NCSA [see *access*, Spring 1993]. Their program plots the Mandelbrot set (named after Benoit Mandelbrot) by means of a calculation that is repeated recursively until the result is greater than 2. Based on the number of times the calculation can be performed until it "blows up" (i.e., produces a number greater than 2), different colors are assigned to each pixel location on a computer monitor.

The calculation used in the Mandelbrot set takes a complex number, represented in the form of a point on a graph—one coordinate

is a real number and the other an imaginary one—which corresponds to a pixel location. This number is squared and then added to its original value. The result of this calculation is squared, then added to the original value, and this process is repeated until a number greater than 2 is produced. As many as a billion calculations may be needed to generate a single image.

Running Fractal Microscope

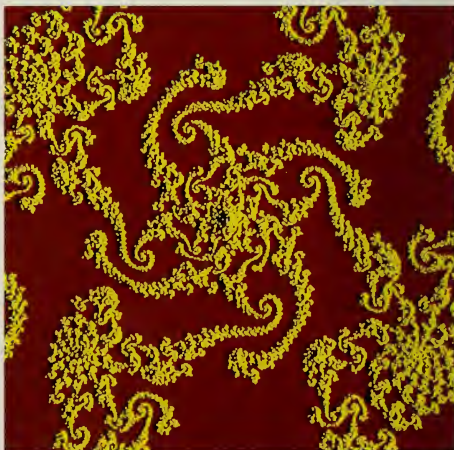
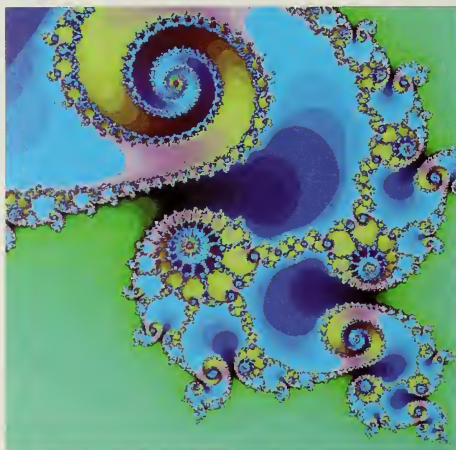
Students can zoom in on portions of the Mandelbrot set and view new images. With only minor promptings by the teacher on how to view the image to find where patterns can be observed, students can explore on their own. The program can be used to explore addition, multiplication, symmetry, and infinity; for more advanced students, more complex patterns can be introduced.

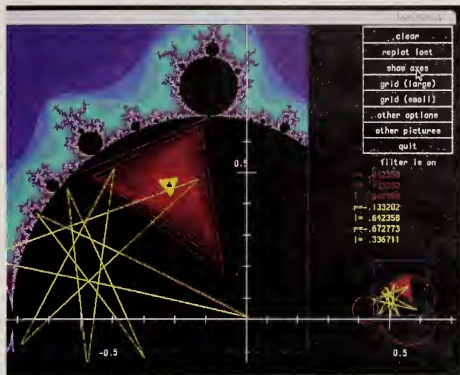
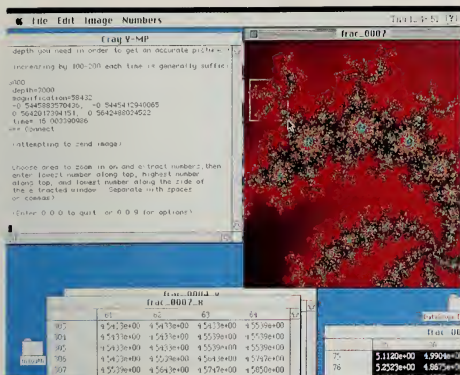
Running the Fractal Microscope program with a supercomputer allows results to be viewed in a matter of seconds—or minutes, for extremely magnified images. By comparison,

many of the images would take hours just to plot on a microcomputer, making the activity impractical for a classroom setting. Speed enabled by the ISDN link makes it possible for teachers to get students interested in math by rapidly creating attention-grabbing fractal images. Teachers then use the images to illustrate the concepts they want to convey.

Fractal Microscope is only one of many software programs NCSA's Education Group uses with schools. Others include Chem Viz [see *access*, May–June 1992], Interactive Galaxy Simulation, and Biology Explorer. Plans are already underway to create documents using NCSA Mosaic [see *access*, Spring 1993] for next fall. ▲

Part of the Mandelbrot set, generated with Fractal Microscope. Created by Michael South, REU student, and Robert Panoff, mentor. (Courtesy of NCSA Education Program)





Students at NCSA's SuperQuest Summer Institute with Larry Smarr. Those attending were from Bob Jones High School, Madison, AL; Illinois Mathematics and Science Academy, Aurora, IL; Riverside University High School, Milwaukee, WI; and Montgomery Blair High School, Silver Spring, MD. (Photo by Thompson-McClellan Photography)

Claremont High wins award

The Claremont High School team won second place in the SuperQuest '92 Best Student Paper Competition, which took place after the research projects were completed. Their project was to verify and expand topological knot tables.

Team members were Christopher Candy, Kaan Erdener, and Danny Wu; Robs Muir was their teacher-coach. They participated in SuperQuest '92 at NCSA [see *access*, July–September 1992].

Sponsors of the SuperQuest program are the National Science Foundation, Digital Equipment Corporation, Cornell Theory Center, NCSA, Alabama Supercomputer Network, University of Alabama–Huntsville, Oregon Graduate Institute, Reed College, Sandia National Laboratory, IBM Corporation, Cray Research Inc., Intel Corporation, Cisco Inc., and the Advanced Digital Communications Consortium.

(Left) Fractal Microscope in use.

(Right) Orbits of points in the Mandelbrot set plotted by StarStruck. (Courtesy of NCSA Education Program)

1993–94 REU members

Eight students, who have been chosen to participate in NCSA's Research Experiences for Undergraduates (REU) program [see *access*, Spring 1993], are listed below in order of students, academic affiliations, and NCSA mentors. All appointments were approved by NSF.

- William D. Baker, Jr., Univ. of Tulsa (Vernon Burton and Barbara Mihalas)
- Amy Biermann, Bryn Mawr College (Michael Heath and Robert Panoff)
- Stephen G. Gaddy, Penn. State Univ. (Robert Wilhelmson)
- Tejas R. Katwala, NJ Inst. of Technology (Barbara Mihalas)
- Stephen E. Lamm, Univ. of California at Irvine (Michael Heath and Robert Wilhelmson)
- Ed Mlodzik, Creighton Univ. (Robert Wilhelmson)
- J. Michael Pauza, Univ. of Tennessee at Chattanooga (Ed Seidel)
- Indira Rao, Univ. of Nevada at Reno (Shankar Subramaniam)

HP, CONVEX TEAM WITH NCSA . . . FOR SCALABLE APPLICATIONS RESEARCH

On June 1, Hewlett-Packard Company, Convex Computer Corporation, and NCSA announced a collaborative effort built on a cluster of high-performance Hewlett-Packard (HP) workstations and a Convex supercomputer.

The HP/Convex cluster will be used by researchers for scalable application development. HP workstations at NCSA's site also will be used in the research and development of distributed-computing environments, distributed and parallel applications, and multimedia applications.

HP is providing more than \$1 million of equipment to NCSA, including 18 desktop and desksize HP Apollo 9000 Series 700 workstations and multimedia software. The cluster will be tightly integrated with a CONVEX C3880 supercomputer creating a Meta Series using a high-performance interconnect and Convex software to generate the highest levels of application throughput performance. NCSA's users will access the cluster to carry out advanced scientific research in engineering, biology, materials and earth sciences, gas dynamics, computational chemistry, and seismic analysis.

The HP/Convex cluster is a major component of NCSA's metacomputer, a collection of supercomputers, workstations, data storage, and advanced imaging resources that are integrated via sophisticated software technology to give users an environment that is as straightforward to use as a single computer [see *access*, September–December 1991]. The new cluster will spur NCSA efforts to build a scalable metacomputer based on leading-edge RISC technologies.

NCSA and the other three NSF centers—Cornell Theory Center, Pittsburgh Supercomputing Center, and San Diego Supercomputer Center—are extending the metacomputer

concept to the National MetaCenter, a synthesis of the intellectual and computing resources of the four centers [see *access*, October–December 1992].

HP, Convex continue alliance

The announcement strengthens the business and technology alliance between HP and Convex. In May, HP announced it will license to Convex its UNIX-based HP-UX1 operating system and related software technologies; Convex will license to HP current and future software technologies. Previously, Convex has announced that it will base its future scalable parallel-processing system (SPP) on HP's PA-RISC2 technology.

HP and Convex, in their partnership with NCSA, believe they can lead the market in the development of scalable computers, which provide several advantages over traditional high-end machines. Scalable computers are modular, upgradable, and binary-compatible from desktop to supercomputer, making them more economical and flexible than traditional supercomputers.

Because Convex's SPP system, expected to be available in mid-1994, will be binary-compatible with HP's PA-RISC processors, users will have access to more than 4,000 PA-RISC-based applications addressing a broad spectrum of scientific and engineering disciplines. In addition, the SPP system will be source-compatible with existing CONVEX C Series supercomputers so that customers can use the 1,300 third-party applications already running on Convex's current product line.

"This joint effort is further testimony to HP's status as the leading supplier of workstations to the scientific and engineering communities," says Gary B. Eichhorn, general manager of HP's Workstation Systems

Group. "We're confident that the work the National MetaCenter is doing through NCSA and its other sites will one day fundamentally change the way we live our daily lives—at work and at home. HP is looking forward to this comprehensive, long-term partnership with NCSA, our continuing relationship with Convex, and to playing a key role in the development of the information infrastructure of tomorrow."

"The future of high-performance computing depends on the development and availability of software applications that are able to take advantage of the latest hardware advances," said Steven J. Wallach, Convex's senior vice president of technology. "We are pleased to col-



laborate with NCSA, a recognized leader in development of supercomputer applications, and to advance computer research in existing areas such as the national data highway. This effort further demonstrates the strength of Convex's partnership with HP and our commitment to PA-RISC technology on our current high-performance systems.

Corporate participation

As part of a separate effort, the HP/Convex cluster will be used as a distributed-computing testbed for a new corporate "participation" program at NCSA. The program will allow corporations to join NCSA, HP, and Convex in developing distributed-computing environments and services and to port and optimize their application codes for the HP/Convex scalable platforms.

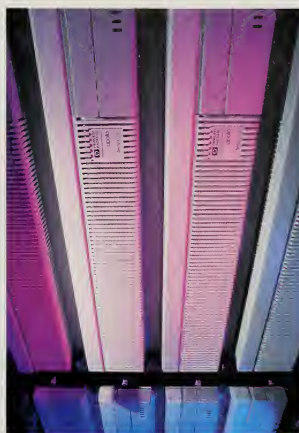
"We view the participation program as a strong new component to our Industrial Program, allowing partners to move toward scalable computing in a structured way in collaboration with our staff," said John Stevenson, NCSA corporate officer. The center's industrial partners include AT&T, Caterpillar, Dow Chemical, Eli Lilly, FMC, Kodak, J. P. Morgan, Motorola, Phillips

Petroleum, Schlumberger, and United Technologies.

Collaborative technologies

NCSA will use several of the HP workstations in its Collaboratorium research laboratory, which is for developing new collaborative hypermedia and multimedia-based technologies. NCSA's globally distributed hypermedia software system, NCSA Mosaic, provides a user interface to the Internet and expanding corporate networks [see *access*, Spring 1993]. This type of next-generation electronic information system, in concert with HP- and NCSA-developed digital conferencing systems, provides the foundation for globally networked information and data solutions and the infrastructure for agile manufacturing efforts by HP and NCSA's clients.

"The combination of HP workstations and Convex supercomputer technology is a key move toward realizing NCSA's goal of seamless desktop-to-teraflop capabilities," says NCSA Director Larry Smarr. "The wealth of third-party software programs available on these systems provides us with an excellent environment for real-world science and engineering problems." ▲



NCSA's deskside HP Apollo 9000 cluster (opposite page) and close-up.

(Photos by Wilmer Zehr)

HIGH DEFINITION TECHNOLOGIES AT NCSA

BY VINCENT JURGENS, TECHNICAL SERVICES, SCIENTIFIC COMMUNICATION AND MEDIA SERVICES

The advancement of computational science, and the related hardware, moves forward with a general increase in information handling capabilities. At the end of the process is a presentation of the data, whether it is in text, numeric, visual, and/or audio forms.

The visual analog to higher powered computers, networks, and storage devices is High Definition (HD) video technologies. NCSA is building an HD facility which is flexible enough to encompass the already high-resolution displays users are accustomed to in workstations, along with alternative display resolutions and new HDTV, recordable video resolutions. The equipment will be hardwired into the HIPPI network being established for all of NCSA's high-performance machines.

First phase of HD

The first phase of the HD facility puts a PsiTech HFB24 multiresolution frame buffer on our HIPPI network, feeding a 100" rear-screen projected, Barco 1200 multisync projector.

The CRAY Y/MP, CONVEX C3380, Thinking Machines' CM-5, and SGI Onyx computer systems will eventually all be on the HIPPI network and have PsiTech drivers installed for users to work with.

Maximum resolution is 2048 x 2048 pixels, at 60 Hz, progressive scan refresh rates. This is a much higher resolution than any current HDTV standards or proposals. Being multiresolution, however, both the frame buffer and projector can be used at various resolutions, from 1280 x 1024 at 120 Hz on up. Any new standards for American HDTV production can be programmed into the PsiTech in the future.

HD's future at NCSA

The future directions of HD at NCSA involve the development of a true HD video and audio production environment, including recording, manipulation, and editing, building upon our experience with digital NTSC post-

HD continued on page 33

REMODELING A CAREER

BY PAULETTE SANCKEN, NCSA PUBLIC INFORMATION SPECIALIST

Talking with David Bennett is a great way to jump-start a day. His enthusiasm for his job and the story of his recent life overhaul is enough to make one consider a midlife career change as advantageous.

Bennett's career shift began when he discovered the realm of scientific visualization while attending an open house at UIUC's Beckman Institute in 1988. Viewing computer images created by Donna Cox and Ray Idaszak started a mental journey that culminated with Bennett quitting his job as a business systems director at an extended care facility and going back to school—at age 41. (Cox is NCSA co-director of SCMS and UIUC professor of Art; Idaszak, manager of High Performance Technology at the Information Technology Division of MCNC, was once a scientific visualization specialist at NCSA.)

Bennett's timing could not have been better. Parkland Community College was initiating a curriculum in visualization computer graphics [see *access*, May–June 1989]. He became one of the first to enter the program. (Parkland now offers an associate in applied science career program in visualization computer graphics.)

After two years of full-time study, part-time work, and an internship with NCSA industrial partner Motorola, Bennett was ready to re-enter the work force.

Off to NCSC and AVS

In August 1990, Bennett started a new job as a scientific visualization specialist I at the North Carolina Supercomputing Center (NCSC). Within a year, he was promoted to a visualization specialist II working with AVS (Application Visualization System) software and was made project leader of the International AVS Center (IAC) located at MCNC. Another promotion propelled him to manager of Strategic Programs; today his official title is manager of Technical Program Development.



Vision Dome—one of many projects initiated by David Bennett, IAC. (Courtesy of AVS; visualization by Chris Landreth, MCNC Senior Scientific Animator)

All accomplished just short of three years—which is not surprising as you listen to the enthusiasm and obviously innate curiosity that comes from Bennett's voice and choice of words: "I have this sort of hunger. And because of that, I want to find out about new things. I go out, absorb as much as possible, and get a good overview. . . . Finding out what is going on in the world has led to lots of other interesting developments [here at the center]."

One such development is the AVS '93 Conference held in May 1993 at Orlando, FL. As coordinator of the conference, Bennett invited NCSA Director Larry Smarr to give the keynote speech. "When I did the introduction," Bennett reflects, "I thanked him. Without his blessing of the [Parkland] program—as well as Donna Cox's—I would probably still be out there selling shoes, or pumping gas, or no telling what. So I was really pleased that NCSA was willing to open their doors to a bunch of students who did not know what

the heck they were doing, on some totally innovative program that had never been tried anywhere else. [NCSA and Parkland] had no idea whether it was going to succeed. This is the sort of thing that your kind of center should be doing—promoting those leading-edge innovations. Taking them forward, and then at some point passing the gauntlet on for others to carry forward."

Smarr's conference address focused on metacomputing and AVS. "AVS is typically thought of as a stand-alone workstation visualization tool," says Smarr. "This limits the size of datasets one can fit on a workstation, as well as the turnaround time being limited by the speed of the workstation." He suggests that by using AVS as a client-server, one could utilize the National Meta-center's HPCC machines as nationwide visualization servers.

For more information about AVS, see "AVS simplifies visualization" on the opposite page.

Rounding out the circle

Bennett's enthusiasm about visualization continues. Two years ago a program, similar to Parkland's, rose out of a conversation between Bennett and visitors from North Carolina's Wake Technical Community College. Interested in this new technology, college officials wanted to know what they could do to prepare their students for opportunities in the scientific visualization field. Bennett suggested the creation of a program like the one he graduated from at Parkland.

This fall, Wake College will offer its first associate degree program in scientific visualization, which filled up just weeks after the announcement. If David Bennett is an example, graduates can expect a career that will only be limited by their own dreams. ▲

AVS simplifies visualization

Distributed by Advanced Visual Systems Inc., Application Visualization System (AVS) is a scientific visualization and application development environment tool that enables users to construct visualizations from generic modules within the software. Built on a data flow paradigm, the easy-to-use graphical interface connects modules that result in the proper process for generating images.

Bridging platforms AVS is useful to researchers because many people can use the same techniques and generic AVS modules even though they may be in different fields. AVS allows users to bridge platforms, or run any of its modules on any machine that has AVS installed. It is a distributed, heterogeneous, collaborative software tool. Several popular modules developed by users and distributed by the International AVS Center (IAC) utilize the Data Transfer Mechanism (DTM) protocol as a collaborative tool in the AVS environment. DTM was developed at NCSA by Jeff Terstieper, research programmer in the Computing and Communications Group [see *access*, September–December 1991].

Customizing modules "There are certain stages to the visualization process like reading in the data, scaling the data to fit in a certain range, associating colors with the numbers, or perhaps making a geometric form from the numbers. With AVS, every separate stage of this process is written as a module," explains William (Bill) Sherman, NCSA Virtual Reality project leader. With AVS, users can write new modules to be used with the modules built into AVS. For example, NCSA's PATHFINDER Program, being developed by NCSA Research Scientist Robert Wilhemson, is a collection of such modules that runs on several SGIs and on the CONVEX C3 using AVS [see *access*, July–September 1992]. NCSA Principal Investigator Joseph Lyding is running AVS on an HP system in his lab (see page 4).

International AVS Center The IAC serves as a catalyst for expanding the AVS user base. It fosters discipline-specific module development and new uses for AVS. This worldwide clearinghouse collects, ports, and distributes user-contributed, public domain modules and acts as liaison between users and vendors. Advanced Visual Systems Inc., Convex Computer Corp., Digital Equipment Corp., Hewlett-Packard Co., IBM, Kubota Pacific Corp., and SUN Microsystems Inc., fund the IAC and promote software development. IAC publishes a quarterly journal called *AVS Network News*, hosts a yearly AVS User Group Conference, maintains an AVS Showroom, maintains a newsgroup (comp.graphics.avs), and presents lectures to user groups in Europe, Japan, and the U.S.

For more information, contact the International AVS Center, P. O. Box 12889, 3021 Cornwallis Road, Research Triangle Park, NC 27709-2889 (U.S. mail); avs@ncsa.uiuc.edu (electronic mail); (919) 248-1100 (phone); (919) 248-1101 (facsimile).

NOTE: Randall Graham, science writer, contributed to this sidebar.

HD continued from page 31

production and the creation of an HD animation for SIGGRAPH '92.

Other forms of HD workstations, whereby HD displays are used as the main interface to one's workstation, are also being explored.

To facilitate integration of our onsite resources, a comprehensive infrastructure is being planned, including video routing, scan conversion (between numerous video standards), recording, and display devices.

Users are invited to visit the facility and explore the ways they might use this High Definition facility. Contact Vincent Jurgens, by phone at (217) 244-1543 or by electronic mail at vjurgens@ncsa.uiuc.edu (Internet). ▲

NCSA MOSAIC EXPLOITS INTERNET

BY KENNETH CHANG, NCSA

RESEARCH PROGRAMMER, PUBLICATIONS GROUP

Click. Click. See an exhibit of dinosaur fossils on your computer screen. *Click. Click.* Listen to a half-hour speech by F.W. DeKlerk to the National Press Club. *Click. Click.* Watch a short movie showing the path of last year's Hurricane Bob.

The age of a global information network arrived some time ago, but few noticed, because there was no easy way to navigate through the nearly 10 terabytes of information—about 10,000 times more data than is found on a typical PC hard disk—that is publicly available on the Internet computer network.

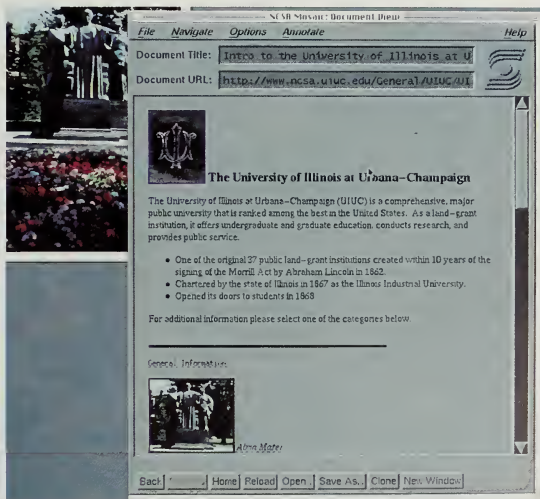
NCSA Mosaic, the latest software offering from NCSA's Software Development Group, opens a portal to this cornucopia with a few clicks of the mouse.

Click. Click. Read the text of a recent Supreme Court decision. *Click. Click.* Examine the latest satellite picture from the U.S. Weather Service. *Click. Click.* Browse through the electronic version of *access*.

Built atop the World Wide Web technology developed by CERN (the high-energy physics laboratory in Switzerland), NCSA Mosaic is, in essence, HyperCard on a global scale. Each phrase highlighted in blue is a link pointing to related information, which can include text, images, sounds, and video sequences. For example, clicking on the

Mosaic continued on page 37

Mosaic screen shot.



THE WHOLE INTERNET

USER'S GUIDE AND CATALOG

BY PAULETTE SANCKEN, NCSA PUBLIC INFORMATION SPECIALIST, PUBLICATIONS GROUP



When asked to review Ed Krol's *The Whole Internet User's Guide and Catalog*, I balked. Me? Read a technical book with the notion of understanding it well enough to tell others? I had played around in cyberspace enough to know there's a lot of information out there—with seemingly many ways to view it—and it amounted to a confusing system only the “techno-geek” could embrace. But, okay, why not? I was certainly interested enough to give it a go.

My misgivings turned out to be insignificant. The book is a surprisingly good read. It's well written and understandable to the novice; I would expect the experienced user to also benefit. “This book is intended for anyone who wants access to the Internet's tremendous resources. It's a book for professionals, certainly, but not computer professionals. It's designed for those who want to use the network, but who don't want to become a professional networker in order to use it,” states Krol in his preface.

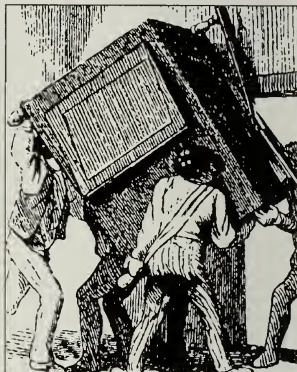
How the book is organized

Krol starts out with some history and theory, promising to keep it to a minimum—which he does. Most of the book discusses how to use the tools that allow your computer to do things on the Internet: moving files with FTP, using electronic mail, accessing network news, working with Archie, and how to find someone on the system. And there are several chapters devoted to the most recent, “friendly” tools like Gopher, WAIS, and the World-Wide Web. The final section is a *Resource Catalog*—a list of things Krol and some helpers found on the Internet. Arranged by subject, it's a great place to start to investigate what's available.

Can't afford a magazine subscription? Login to the electronic version of *PC Magazine* published by Ziff Davis (see page 293). Having special guests for dinner tonight? There's a recipe archive to browse through (see page 295). Developing Carpal Tunnel Syndrome from too much Internet browsing? Try the FDA Electronic Bulletin Board for information (see page 301). Want to play chess with another user? Find out what others think about a recent movie? It's all there, and more.

Krol writes “You need three things to explore and use the Internet: a desire for information, the ability to use a computer, and access to the Internet. Desire for information is the most important.”

I might add that you need a fourth: a means to understand the workings of the Internet. Krol's book certainly provides this vital link. If you are interested in the Internet, but you are not willing to work your way through a mass of technical jargon and oblique explanations, this



Illustrations from “Preface” (left) and “Moving Files: FTP” (right) in *The Whole Internet User's Guide and Catalog*. (Courtesy of O'Reilly & Associates Inc.)

book is for you. It's available in most bookstores. It is published by O'Reilly & Associates Inc., Sebastopol, CA.

About the author

Krol was NCSA's network manager in its early days. His original task was to get the UIUC campus connected to ARPAnet, which was the beginning of his work in wide-area networking. He also oversaw the UIUC installation of NSFNET, and he now works at Computing and Communications Services Office directing network operations and network information services for the campus. ▲

CENTER CACHE

Awards

Charles Catlett, associate director for Computing and Communications, received the IEEE Communications Society's Fred W. Ellersick Prize Paper Award for 1992, which will be presented at the Globecom Conference, November 29-December 2, 1993. The paper, "In Search of Gigabit Applications," was published in the April 1992 issue of IEEE's *Communications Magazine*.

Outreach

Michael Heath, leader of NCSA's Mathematics and Computer Science team in the Applications Group, was named co-chair for Algorithms on the Program Committee for the 5th Symposium on Frontiers of Massively Parallel Computation that will be held in McLean, VA, June 1994.

Alaina Kanfer, social science research assistant; **Michael Welge**, research programmer; and **Scott Lathrop**, team leader, have been working with the Applications and Technical Subcommittees of the Champaign County Chamber of Commerce's Infrastructure Task Force.

The subcommittees are defining and investigating local needs in education, agribusiness, health care, community services, local government, and small business applications in response to NCSA Director Larry Smarr's challenge for-Champaign-Urbana to take advantage of emerging technologies [see *access*, Spring 1993].

NCSA has been working to support Champaign-Urbana's FreeNet effort called PrairieNet, which will coordinate with the chamber's activities.

Personnel

Beth Richardson, NCSA senior research programmer, began working with Alan Craig on NCSA's Training in mid-July and is now a member of NCSA's User Services. She continues to provide individual assistance to users by spending part of her time in the Consulting Office.

Balaji Veeraraghavan

recently joined NCSA's Applications Group as a research programmer in computational chemistry. **Jay Alameda**, formerly Dow Chemical Co.'s consultant, joined the group as a research programmer in chemical engineering.

Prasad Ravi took Alameda's former position as Dow consultant.

Promotion

Donna Cox, co-director of NCSA's Scientific Communication and Media Services, was recently promoted to professor of art and design by the UI Board of Trustees. Computer graphic artist Cox teaches in the UIUC College of Fine and Applied Arts.

Publication

As *access* was in the final phase of production, the announcement was made that a group of UIUC chemists had created a 3D model that may predict where hormonal steroids bind to proteins. The researchers used NCSA's CRAY-2 system and an SGI Crimson

workstation at the UIUC Department of Chemistry to model their calculations.

The group's leader

Peter Wolynes, NCSA principal investigator, UIUC chemistry professor, and member of the Beckman Institute, made the announcement at the annual meeting of the American Chemical Society at Chicago in mid-August. The model will be published in the October *Proceedings of the National Academy of Sciences*.

Other members of the research team include **John Katzenellbogen**, UIUC professor of chemistry, and **Zan Luthey-Schulten**, UIUC chemist and NCSA research scientist.

Visitor

Thomas DeFanti, co-director of UIC's Electronic Visualization Laboratory, is a Visiting Associate Director for Virtual Environments at NCSA during the fall semester of the 1993-94 academic year. While on sabbatical to NCSA, DeFanti will be collaborating with NCSA's Visualization Task Force to build a leading-edge virtual environment facility.

▲

NICO HABERMANN (1932-1993)

A. Nico Habermann, NSF assistant director for computer and information science and engineering, suffered a fatal heart attack at his home in Pittsburgh, PA on August 8. He was 62.

Since 1991, Habermann had been on leave to NSF from Carnegie Mellon University. At Carnegie Mellon, Habermann was the Alan J. Perlis professor of computer science and founder of the Software Engineering Institute there.

An internationally known computer scientist, Habermann was recognized for his work in programming languages, operating systems, software engineering, and packages. Born in the Netherlands, he was educated at the Free University of Amsterdam before obtaining his doctorate in applied mathematics from the Technological University at Eindhoven.

He is survived by his wife and four children.

The directors and staff of NCSA extend their sympathy to the Habermann family. Habermann's passing is a great loss to the NSF centers since he guided them in the development of the National MetaCenter. ▲



NCSA and SDSC collaborated to hold simultaneous MetaCenter Computational Science Institutes on Parallel Computing in August. Two sessions were held jointly via the medium of videoteleconferencing. Those who participated are pictured at the Beckman Institute. (Photo by Tony Baylis, SCMS)

HCI PAPERS AVAILABLE BY COLLEEN BUSHELL,
VISUALIZATION AND HUMAN-COMPUTER INTERACTION
DEVELOPER, SOFTWARE DEVELOPMENT GROUP

NCSA sponsors a special interest group in Human-Computer Interaction (HCI) [see access, October-December 1992]. This group, chaired by Colleen Bushell, meets twice monthly during the academic year to present current research and development activities. Areas of discussion include technical, sociological, psychological, and aesthetic issues of human-computer interaction. They range over collaborative technologies, visualization, virtual reality, information systems, and multimedia. The group is open to the campus community and currently consists of approximately 60 people representing 16 UIUC departments.

For additional information about the HCI group, contact Colleen Bushell at (217) 244-6830 via phone or cbushell@ncsa.uiuc.edu via Internet. Announcements for HCI meetings/presentations are posted in the UIUC newsgroup: ncsa.hci.uiuc (Internet).

NCSA has made available papers written by HCI group members in its technical report series. The 1992-93 academic year offering, called *HCI Papers: Compilation for 1992-93*, will be collected together as a single report. Additional papers will be added to the collection each semester. Reports that may be accessed soon from the NCSA servers are marked with an asterisk (*). (See the inside back cover for the addresses of the servers.) Following is a list of papers that will be available in the near future:

M. Pauline Baker "Exploring the Relationship between User Task and Display Parameters in Support of Visual Data Analysis" *

Noshir S. Contractor and David R. Seibold "Theoretical Framework for the Study of Structuring Processes in Group Decision Support Systems: Adaptive Structuration Theory and Self-Organizing Systems Theory"
 [Originally in *Human Communication Research*, vol. 19, no. 4 (June 1993)]

Patricia M. Jones "Dimensions of Human-Computer Cooperative Problem Solving" *

Barbara J. O'Keefe, Noshir S. Contractor, Patricia M. Jones, and Stephen C-Y. Lu "Studying and Supporting Human Interaction Processes" *

Carla Scaletti and Alan B. Craig "Using Sound to Extract Meaning from Complex Data"
 [Originally in "Extracting Meaning from Complex Data: Processing, Display, Interaction II," Edward J. Farrell (Ed.), *Proc. SPIE 1459*, 207-219 (1991)]

Susan Leigh Star "The Trojan Door: Organizations, Work, and the 'Open Black Box'" *
 [Originally in *Systems/Practice*, vol. 5 (1992)]

Susan Leigh Star "Cooperation without Consensus in Scientific Problem Solving: Dynamics of Closure in Open Systems" *

[Originally in *CSCW: Cooperation or Conflict?* Steve Easterbrook (Ed.), 93-105. London: Springer-Verlag (1993).]

Susan Leigh Star and Geoffrey Bowker "Knowledge and Infrastructure in International Information Management: Problems of Classification and Coding" *

[To appear in *Information Acumen: The Understanding and Use of Knowledge in Modern Business*, L. Bud (Ed.). London: Routledge (1993).]

Christopher D. Wickens "Cognitive Issues in Virtual Reality" *

[To appear in *Virtual Reality*, W. Barfield and T. Furness (Eds.)]

Christopher D. Wickens "Virtual Reality in Education" *

[To appear in *Proc. IEEE Internatl. Conf. on Systems, Man, and Cybernetics* (1992).]

Christopher D. Wickens and David H. Merwin "Visualization of Higher Dimensional Databases" *

[Originally in *Proc. IEEE Visualization Conf.* (1992)]

Christopher D. Wickens, David H. Merwin, and Emilie L. Lin "Human Factors Implications of Graphics Enhancements for the Visualization of Scientific Data: Dimensional Integrality, Stereopsis, Motion, and Mesh" *

These papers soon may be obtained through the NCSA *Technical Resource Catalog* or by contacting Orders for Publications, NCSA Software, and Multimedia [see **ncsa contacts**, page 2]. ▲



UniTree, NCSA's new archival storage system that replaced the Common File System (CFS), and the Andrew File System (AFS), NCSA's new distributed file system, are overseen by the Distributed File Systems and Mass Storage team of (left to right) Michelle Butler, Jeff Rosendale, Ral Geis, Arlan Finstead, and Nancy Yeager (center). (Photo by Tony Baylis, SCMS)

Mosaic continued from page 33

words "dinosaur exhibit" could send you zipping through cyberspace to the exhibit on dinosaur fossils put together at Honolulu Community College.

"Mosaic is turning hypermedia into a medium that can be practically used," says Marc Andreessen, NCSA programmer of the X Windows System version of Mosaic. "It's kind of like a '90s NCSA Telnet. Instead of logging into another computer, all of these computers on the network are able to give you information."

NCSA Mosaic for the X Windows System was released in April. Since then, 5,000 copies a month have been downloaded from NCSA's anonymous ftp server. By the time you read this, Version 2.0 should be available, as should versions for the Macintosh and Microsoft Windows.

NCSA Mosaic offers access to the more than 200 World Wide Web Servers, approximately 1,000 Gopher servers, and thousands of ftp servers, as well as WAIS databases and more obscure protocols. One of the greatest advantages of Mosaic, though, is that it combines all of these varied information servers into one unified information space. (That is, one rarely needs to know more than "click on the colored text" to effectively use the software.) In addition, Mosaic's Annotations feature enables one to attach personal notes to a document.

Applications for this new technology are still in the discovery stage. The National Consortium for High Performance Computing [see *access*, Spring 1993] plans a Digital Library and Informations Systems Testbed, which

will include such projects as an online library of medical images for the Human Genome and Human Brain Projects, archives of data from environmental monitoring satellites, and large datasets for social science research. Mosaic could be the software of choice for the testbed.

"NCSA Mosaic is driving the next stage of evolution of the global Internet," says Joseph Hardin, head of the NCSA Software Development Group. "What emerges will be a new form of life online."

NCSA Mosaic is available via anonymous ftp from NCSA's ftp server. See the inside back cover for directions on how to access the ftp server from the Internet.

This software is free for individual use, but is copyrighted by the University of Illinois. NCSA and the University of Illinois retain rights to restrict the modification and redistribution of this software. ▲

ACM/SAC '94

Phoenix, AZ is the location of the 1994 ACM Symposium on Applied Computing (SAC '94) to be held March 6-8 at the Phoenix Civic Plaza.

For the past nine years, SAC has been a primary forum for applied computing practitioners and researchers in the areas related to genetic algorithms and other optimization techniques. The conference will be held in conjunction with the 1994 ACM Computer Science Conference (CSC '94).

For further information, contact the conference coordinator, Edmund Deaton of San Diego State University at deaton@cs.sdsu.edu (Internet).

NCSA PREPRINTS AND TECHNICAL REPORTS BY GINNY HUDAK-DAVID, NCSA PUBLICATIONS EDITOR, PUBLICATIONS GROUP

Last year NCSA established a preprint and a technical report series to showcase the work of NCSA staff. Below are listed the preprints and reports processed to date. Reports and preprints that are accessible on the NCSA servers (anonymous FTP and the World Wide Web) are noted with an asterisk (*). See the inside back cover for the addresses of the servers.

Preprints

P001 **Andrew Abrahams, David Bernstein, David Hobill, Edward Seidel, and Larry Smarr** "Numerically Generated Black Hole Spacetimes: Interaction with Gravitational Waves" (February 1992)*

P002 **James M. Stone and Michael L. Norman** "The Magnetic Collimation of Bipolar Outflows I: Adiabatic Simulations" (April 1992)*

P003 **James M. Stone and Michael L. Norman** "ZEUS-2D: A Radiation Magnetohydrodynamics Code for Astrophysical Flows in Two Space Dimensions: I. The Hydrodynamic Algorithms and Tests" (April 1992)*

P004 **James M. Stone and Michael L. Norman** "ZEUS-2D: A Radiation Magnetohydrodynamics Code for Astrophysical Flows in Two Space Dimensions: II. The Magnetohydrodynamic Algorithms and Tests" (April 1992)*

P005 **James M. Stone, Dimitri Mihalas, and Michael L. Norman** "ZEUS-2D: A Radiation Magnetohydrodynamics Code for Astrophysical Flows in Two Space Dimensions: III. The Radiation Hydrodynamic Algorithms and Tests" (April 1992)*

CRAY-2 stops. NCSA's CRAY-2 system was unplugged after NCSA Director Larry Smarr typed the command for shutdown on August 26. The CRAY-2 was installed in 1988. (Left to right) Bob Wilhemson, Mike Norman, Jim Bottum, Charlie Catlett, Jeff Rosendale, and Smarr. (Photo by Tony Baylis, SCMS)



P006 **James M. Stone and Michael L. Norman** "The 3D Interaction of a Supernova Remnant with an Interstellar Cloud" (April 1992)*

P007 **James M. Stone and Dimitri Mihalas** "Upwind Monotonic Interpolation Methods for the Solution of the Time Dependent Radiative Transfer Equation" (April 1992)*

P008 **James M. Stone, John F. Hawley, Charles R. Evans, and Michael L. Norman** "A Test Suite for Magnetohydrodynamical Simulations" (April 1992)*

P009 **Harrell Sellers** "Kinetic Isolation: An Efficient Method for Constrained Geometry Optimization" (April 1992)

P010 **Harrell Sellers** "The C2-DIIS Convergence Acceleration Algorithm" (April 1992)

P011 **Michael L. Norman and Dinshaw Balsara** "3D Hydrodynamical Simulations of Extragalactic Jets" (April 1992)

P012 **Louis J. Wicker and Robert B. Wilhelmson** "Numerical Simulation of Tornadoogenesis within a Supercell Thunderstorm" (May 1992)

P013 **Mordecai-Mark Mac Low and Michael L. Norman** "Nonlinear Growth of Dynamical Overstabilities in Blast Waves" (July 1992)

P014 **Sung Yi, Gerry D. Pollack, M. Fouad Ahmad, and Harry H. Hilton** "Thermo-viscoelastic Finite Element Analysis of Composite Shells" (September 1992)

P015 **M. H. Swellam, M. F. Ahmad, R. H. Dodds, and F. V. Lawrence** "The Stress Intensity Factors of Tensile-shear Spot Welds" (September 1992)

P016 **Edward Seidel and Wai-Mo Suen** "Towards a Singular-ity-proof Scheme in Numerical Relativity" (November 1992)

P017 **Amaury Fonseca, Jr. and M. Fouad Ahmad** "PARFES—Parallel Finite Element Solvers for Flow-Induced Fracture" (November 1992)

P018 **Robert B. Wilhelmson, Steve Koch, M. Arrott, J. Hagedorn, G. Mehrotra, C. Shaw, J. Thingvold, B. Jewett, and L. Wicker** "PATHFINDER: Probing Atmospheric Flows in an Interactive and Distributed Environment" (December 1992)

P019 **Keith R. Searight, David P. Wojtowicz, Kenneth P. Bowman, Robert B. Wilhelmson, and John E. Walsh** "Envision: A Collaborative Analysis and Display System for Large Geophysical Data Sets" (December 1992)

P020 **Michael L. Norman** "Magnetic Shaping of SNRs and Their Bubbles" (December 1992)

P021 **Jerry M. Straka, Robert B. Wilhelmson, Louis J. Wicker, John R. Anderson, and Kelvin K. Droegemeier** "Numerical Solutions of a Nonlinear Density Current: A Benchmark Solution and Comparisons" (February 1993)

P022 **Sung Yi, M. Fouad Ahmad, Harry H. Hilton, and Gerry D. Pollock** "Vibration Responses of Viscoelastically Damped Plates" (April 1993)

P023 **Sung Yi, Gerry D. Pollock, M. Fouad Ahmad, and Harry H. Hilton** "Thermo-viscoelastic Analysis of Fiber-matrix Interphase" (April 1993)

P024 **Deyang Song, Eric Golin, and Michael Norman** "A Fine-grain Dataflow Model for Scientific Visualization Systems" (April 1993)*

P025 **Deyang Song and Michael L. Norman** "Cosmic Explorer: A Virtual Reality Environment for Exploring Cosmic Data" (April 1993)*

P026 **Deyang Song and Michael L. Norman** "Visualizing Multiscale Cosmological Data using Virtual Reality" (May 1993)*

P027 **Wenbo Y. Anninos and Michael L. Norman** "Nonlinear Hydrodynamics of Cosmological Sheets I. Numerical Techniques and Tests" (July 1993)*

P028 **Rami M. HajAli, David A. Pecknold, and M. Fouad Ahmad** "Combined Micromechanical and Structural Finite Element Analysis of Laminated Composites" (July 1993)

P029 **Marcus Wagner and David M. Ceperley** "Path Integral Monte Carlo Simulations of H₂ Surfaces" (July 1993)*

P030 **Marcus Wagner and David M. Ceperley** "Path Integral Monte Carlo Simulations of Thin 4He Films on a H₂ Surface" (July 1993)*

P031 **Danesh Tafti** "A Study of High-Order Spatial Finite Difference Formulations for the Incompressible Navier-Stokes Equations" (September 1993)*

P032 **Danesh Tafti** "Vorticity Dynamics and Scalar Transport in Separated and Reattached Flow on a Blunt Plate" (September 1993)*

P033 **Danesh Tafti** "Implementation of a General Purpose Finite-Difference Algorithm on the CM-5 for Direct Numerical Simulations of Turbulence" (September 1993)*

Technical reports

TR001 **Joel Replogle, Charlie Catlett, and Randy Butler** "FDDI Testbed Cray Research/Network Systems Beta Test Results, Revision I" (February 1991)

TR002 **Charles E. Catlett, Domenico Ferrari, Roy Campbell, Larry Landweber, Bill Hibbard, and Murray Thompson** "BLANCA Testbed Annual Progress Report 1990-91" (August 1991)

TR003 **Deyang Song and Michael L. Norman** "Nonlinear Interactive Motion Control Techniques for Virtual Space Navigation" (June 1992)*

TR004 **Greg Bryan** "Adapting CMHOG to Cosmological Studies" (June 1992)*

TR005 **Arlan Finestead and Nancy Yeager** "Performance of a Distributed Superscalar Storage Server" (October 1992)

TR006 **Patrick J. Moran** "A Soft Module Mechanism for Data Flow Systems" (November 1992)

TR008 **Charles E. Catlett, Larry Landweber, et al** "Annual Progress Report 1991-1992 BLANCA Testbed" (December 1992)

TR009 **Charles E. Catlett and Lex Lane** "Experiments in Superscalar RISC Clusters" (December 1992)*

TR010 **Herbert Edelsbrunner and Ping Fu** "Measuring Space Filling Diagrams" (April 1993)

TR011 **Gerry D. Pollock, M. Fouad Ahmad, and Paul Corcoran** "A Finite Element Approach to Landfill Compaction" (April 1993)

TR012 **C. D. Gregory** "A VIEWIT Cookbook for NMR Imaging and Spectroscopy" (April 1993)*

TR013 **Patrick J. Moran** "Nicer-Slicer-Dicer: An Interactive Volume Visualization Tool" (August 1993)*

TR014 **Patrick J. Moran** "Tele-Nicer-Slicer-Dicer: A New Tool for the Visualization of Large Volumetric Data" (August 1993)*

All preprints and technical reports are available free of charge by contacting Orders for Publications, NCSA Software, and Multimedia [see *ncsa contacts*, page 2]. ▲



CSS93. NCSA hosted the 4th annual conference of the Social Science Computing Association's Computing in the Social Sciences 1993 conference in May. Attendees—shown with banquet speaker Cora Marrett (far left), NSF associate director of Sociological, Behavioral, and Economical Sciences directorate—included (left to right) Bruce Tonn, incoming president; Douglas White, outgoing president; and William Bainbridge, head of sociology at NSF and chair of micro-computing, ASA (American Sociological Association). (Photo by Thompson-McClellan Photography)



STUDENTS FROM ST. PETERSBURG

Eleven students plus a couple of their teachers from St. Petersburg, Russia (formerly Leningrad) visited NCSA while in Champaign-Urbana during the spring semester. They participated in an exchange program with University High School as part of a national program that involves 30 high schools around the U.S.

Lex Lane, NCSA system security officer, guided them on a tour of NCSA's Machine Room. Jennifer Czoka, UIUC graduate student in English as a Second Language, acted as their interpreter during the visit.

(Top) Curt Canada of the CM-5 team explained the workings of MPP to the group.



(Bottom) Danilo Smalechko especially was intrigued with the CRAY-2 system. Lex Lane is at his left. (Photos by Thompson-McClellan Photography)

SIGGRAPH '93

SIGGRAPH '93, the 20th of the series, was held August 1-6 in Anaheim, CA. Its theme was "Be a Part of the Vision." Additions to this year's event included the first ACM Multimedia Conference, running concurrently; "Machine Culture: The Virtual Frontier," a curated, interactive art exhibit; and "Designing Technology," displaying "works that explore the role of design in the development of technology."

NCSA's involvement in the conference was as follows:

Panels Committee Chair, Donna Cox, co-director of Scientific Communications & Media Systems (SCMS); Mike McNeill, visualization specialist, committee member; Mark Bajuk, visualization consultant in Applications, committee member.

Courses Robin Bargar, research programmer, Software Development Group, and producer, SCMS, was a lecturer in: "Applied Virtual Reality," an intermediate course on August 2; "An Introduction to Data Sonification," a beginning-level course on August 5.

Electronic Theater "Data Driven: the Story of Franz K." Chris Landreth, North Carolina Supercomputing Center; Robin Bargar, NCSA.

Technical Slide Set "Gravitational Waves from a Strongly Distorted Black Hole." Scientific Research: Peter Anninos, David Bernstein, Ed Seidel, Larry Smarr, NCSA; David Hobill, University of Calgary, Alberta; Scientific Visualization: Mark Bajuk, NCSA [see *access*, May-June 1992].

abbreviations

ARPA	Advanced Research Projects Agency
CRI	Cray Research Inc.
HPCC	High Performance Computing and Communications
MPP	Massively Parallel Processing
NASA	National Aeronautics and Space Administration
NCAR	National Center for Atmospheric Research
NCSA	National Center for Supercomputing Applications
NOAA	National Oceanic and Atmospheric Administration
NRAO	National Radio Astronomy Observatory
NSF	National Science Foundation
TMC	Thinking Machines Corp.
UIC	University of Illinois at Chicago
UIUC	University of Illinois at Urbana-Champaign

documentation orders

Articles in this *access* may refer to items that are available through the NCSA *Technical Resources Catalog*. To receive a copy of the catalog, send your request to Orders for Publication, NCSA Software, and Multimedia [see ncsa contacts, page 2].

accessing NCSA's servers

Many of NCSA's publications (e.g., calendar of events, user guides, *access*, technical reports) as well as SDG software are available via the Internet on one of three NCSA servers: anonymous FTP, Gopher, or the World Wide Web. If you are connected to the Internet, we encourage you to take advantage of the easy-to-use servers to copy or view files.

Anonymous FTP IP address: <ftp.ncsa.uiuc.edu> (141.142.20.50)

Gopher server IP address: <gopher.ncsa.uiuc.edu>

World Wide Web IP address: www.ncsa.uiuc.edu

NCSA WWW home page: <http://www.ncsa.uiuc.edu/General/NCSAHome.html>

If you have any questions about accessing the servers, contact your local system administrator or network expert. Instructions for accessing the anonymous FTP server are below:

downloading from anonymous FTP server

A number of NCSA publications are installed on the NCSA anonymous FTP server. If you are connected to Internet, you can download NCSA publications by following the procedures below. If you have any questions regarding the connection or procedure, consult your local system administrator or network expert.

1. Log on to a host at your site that is connected to Internet and running software supporting the FTP command.
2. Invoke FTP by entering the Internet address of the server: `ftp ftp.ncsa.uiuc.edu` or `ftp 141.142.20.50`
3. Log on using anonymous for the name.
4. Enter your local login name and address (e.g., `smith@ncsa.uiuc.edu`) for the password.
5. Enter `get README.FIRST` to transfer the instructions file (ASCII) to your local host.
6. Enter `quit` to exit FTP and return to your local host.
7. The NCSA publications are located in the `ncsapubs` directory.



access

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152 Computing Applications Building
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Champaign, IL 61820-5518

access

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Spring 1994 vol. 8 no. 1

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Cover: The game of chess acts as a visual metaphor for the competitive drive of scientists engaged in HPCC Grand Challenge research. Each scientist, represented by a game piece, holds a symbol of his/her research area. (Concept and illustration, John Havlik; research, Fran Bond)

It's free!

the CM-5



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termination

WE WISH TO GET YOUR INPUT TO MAKE AN INFORMED DECISION!

NCSA currently provides *access* in print and online via the World Wide Web (WWW). We are evaluating the usefulness of these two formats and seeking reader input. Please send us this card with your input by **July 31, 1994**.

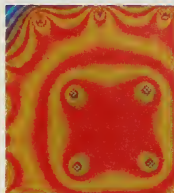
1. Do you have available to you online software such as NCSA Mosaic (Lynx, Cello), which allows you to read HTML files stored on the WWW and view accompanying graphics (gif files)?
- ☐ yes ☐ no

2. Do you currently have a computer available to you that will properly run a program such as NCSA Mosaic? Current minimum system requirements to run the program are listed below.

Unix Workstation
X Windows System

IBM PC
Windows 3.1
80386sx
4 MB memory

Macintosh
System 7
MacTCP
4 MB memory



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- ☐ yes, I have a system with minimum requirements
- ☐ no, I do not have system equipped to run the program

fold here

3. What kind of connection do you have to the Internet?

- ☐ Direct connection
- ☐ Over a modem via SLIP or PPP
- How fast is your modem? ☐ 14.4 K baud ☐ 9600 baud ☐ 1200 or 2400 baud
- ☐ No access to the Internet

4. If NCSA furnished *access* via NCSA Mosaic only (no printed version) would you read it?

- ☐ yes, I prefer to read magazine articles online
- ☐ yes, but not as much as when it was in print
- ☐ no, I do not like reading magazine articles online
- ☐ no (please state why) _____

5. Would providing *access* online only (no printed version) have an impact (good or bad) on your work/research?

- ☐ good impact (please state why) _____
- ☐ bad impact (please state why) _____

6. Please provide any additional comments: _____
- _____
- _____

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ecomputing Applications
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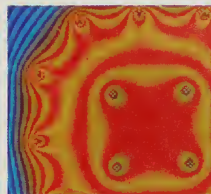
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NOTE: All electronic mail addresses are via Internet.

See inside back cover for details on anonymous FTP, Gopher, and World Wide Web.

CHALLENGING THE FUTURE

Three years ago, a certain class of projects that utilize HPCC support were designated "Grand Challenge" problems. Such problems were recognized for requiring extensive computational capabilities and for being critical to the national interest. In response, a strategy was launched to support R&D efforts that would pursue grand challenges to increase knowledge while serving the nation's economic, security, and educational needs and the global environment. A hallmark of all Grand Challenge projects is that they could not have been attempted until recently because of the previous lack of computational power needed to solve them.

Technological resources have been expanded by this Grand Challenge research through the development of more sophisticated computing and networking to meet scientific demands. This effort has been dubbed the "march to the teraflop" as the search for computing architectures to support such intensive research continues. The goal: a teraflop compute engine that processes a trillion floating point operations per second—about 3,000 times faster than the single processor vector supercomputers of a few years back. Scalable parallel architectures are in the vanguard of this movement. Some recent results on NCSA's scalable machine, the Connection Machine CM-5 may be found on page 4.

Six federally funded Grand Challenge projects—ranging from cosmology to quantum systems (pages 7–14)—that use NCSA's CM-5 and/or other facilities are featured. Their collaborative nature—a requisite due to their intensive demands and sometimes interdisciplinary structure—joins some NCSA research scientists with those at a variety of other institutions.

On page 20, read about industrial partner Schlumberger's research in seismic processing utilizing the CM-5.

NCSA's efforts in transferring technology to the education community (page 21) and the local community (page 37) are featured. Updates on NCSA Mosaic (pages 24 and 25) and the HP cluster (page 26) are included.

This issue's book review focuses on three publications that are available online (page 30).

Two new science writers contributed to this issue—Thomas Krawczyk and Anne Simon Moffat. Victor Ryckaert, student writer, is with NCSA this academic year.

—Fran Bond, Editor



April 22, 1992
CM-5 arrives at NCSA

May 1992

Friendly user
period begins

June 1992

First CM-5 training

August 1992

Sun 4/690 Compile
Server installed

November 1992

First set of Vector
Units installed

December 1992

Complete set of
Vector Units
installed

March 1993

Peer review access
begins

May 1993

Scalable Disk
Array installed

Marching to the teraflop

by Lex Lane, NCSA AD for User Services and Educational Outreach; Radha Nandkumar

With the arrival of Thinking Machine Corporation's CM-5 in the spring of 1992, NCSA committed itself to a fundamental change in its supercomputing strategy. By becoming an early adopter of scalable microprocessor-based technologies, we could work with our users and the computer science community to move to a new architectural paradigm, which promised a historically unprecedented rate of increase in supercomputer speed and memory.

Today, our users are beginning to see the start of this new era. Many of them are sustaining speeds on their codes 200 times faster on the 512-node CM-5 than the national user average on the single processor CRAY Y-MP system, which is used by the majority of NCSA users. Furthermore, the problems CM-5 users can attack are enormously more complex. The monthly average memory has hit 12,800 Mbytes on the 512-node CM-5, which is over 300 times the average memory being used on the CRAY Y-MP. As amazing as these numbers are, one must recall that NCSA's 64-Gflops, 16-Gbyte CM-5, while the largest scalable computer in the Meta-Center, is only one-sixteenth the peak speed of a teraflop machine and has only one-sixty-fourth the memory of a terabyte machine. NCSA's goal is to provide users access to such a machine by 1997-2000.

Getting to this point was not an easy task. Achieving it took a major effort by a broad team of users, computer scientists, Thinking Machine employees, and NCSA staff. The three major stages in this process are reviewed here: The Very Friendly User Phase (May 1992-December 1992), the Friendly User Phase (January 1993-May 1993), and the Production Phase (June 1993-today).

The very friendly user phase
NCSA's 512-node CM-5 arrived April 22, 1992 from Thinking Machines Corporation (TMC), Cambridge, MA. Soon afterwards, various upgrades of its system began (see sidebar, this page).

On delivery, the CM-5 had the expected deficiencies in software and hardware that come with a new model of a leading-edge supercomputer. Missing from the CM-5 hardware were the scaled disk array, the HIPPI network connection, and the all-important vector units. This forced all I/O (disk access, network connections to other machines, etc.) to go through the front-end Suns, which could not provide adequate performance or capacity.

More important for immediate use was the lack of vector units, which accounted for most of the potential for peak performance. Without them, the CM-5 amounted to a collection of Sun workstations, each with modest capacity. While the peak speed per node would be 128 Mflops with the vector units, it was only 5 Mflops without them. This limited the attainable peak performance to about 2.5 Gflops; expected peak vector performance was 64 Gflops.

Nevertheless, a few pioneering CM-5 users were able to begin exploring the use of the machine and gain experience in implementing applications codes. Only after the vector units were installed during November and December 1992 were we able to fully explore the performance potential of the CM-5.

The friendly user phase

With the arrival of the vector units, NCSA decided to aggressively pursue a Strategic Parallelization Program; this program was designed to learn how to rewrite applications to take advantage of the highly parallel architecture. NCSA Director Larry Smarr asked NCSA Research Scientist and UIUC Computer Science faculty member Michael Heath to lead a team of users, Thinking Machines staff, and computer scientists to rewrite a number of academic research codes that would stress various parts of the CM-5's software and hardware. The objective was to learn how to write applications on the CM-5 that would run at least 20% of peak speed, or about 13 Gflops sustained. The time period for achieving this was a few months.

The CM-5 is designed to support both major paradigms for parallel computing: SIMD and MIMD (Single/Multiple Instruction Multiple Data). SIMD is the only paradigm supported by the earlier CM-2. SIMD codes written for the CM-2 can be ported to the CM-5 with little change. Thus, the first codes run on the CM-5 were existing codes written in CM Fortran. (The CM-5 did not yet support C*.) CM Fortran codes had been developed for the CM-2, which had been installed at NCSA in 1989.

Initial runs of such codes on the CM-5—which were disappointingly slow—usually attained only a few Gflops. This performance reflected the immaturity of the CM Fortran compiler for the CM-5, inefficiencies in some key communication primitives (such as *cshift*), and significant differences in the architecture of both machines. This latter aspect required different code structures to reach optimal performance.

Using the CM-5 in MIMD mode requires standard programming languages, FORTRAN 77 or C, combined with explicit message passing to communicate data among processors. The MIMD paradigm is capable of fully exploiting the CM-5's hardware resources because it permits programming techniques such as overlapping communication with computation and better load balancing among processors. However, there is a major impediment to realizing these advantages on the CM-5 because the FORTRAN 77 and C compilers could not generate instructions for the vector units and the compilers did not align arrays in memory to enable vector units to operate on the data. Thus, MIMD message-passing codes were either limited to using only the SPARC processor on each node, or else they had to call assembler coded routines (DPEAC) for vector operations. The former feature severely limits performance, while the latter requires significant overhead to realign data before vectorization can take place—again limiting potential performance.

Early versions of CMMD, the communication library on the CM-5, did not support the “parallel” data layout used by the vector units. For these reasons, initial runs of MIMD codes barely exceeded 1 Gflop.

In response to these constraints, NCSA's Strategic Parallelization Program shifted its focus to improve the performance of SIMD and MIMD codes on the CM-5. This approach required extensive collaboration among research scientists who originally developed the codes, computer scientists who were experienced in parallel architectures and parallel programming, and Thinking Machines personnel who were onsite at NCSA and in Cambridge. Computer scientists helped identify specific bottlenecks that limited code performance [see *access*, January–April, 1992].

Thinking Machines responded to NCSA's experiences and requests by making improvements in compilers, run-time support, communication libraries, and math subroutine libraries. Thinking Machines provided early access to these improvements. For example, Thinking Machines provided some custom-written DPEAC modules and improved supporting utilities for the data realignment required to access them from conventional languages. The ability to handle “parallel” arrays was added to CMMD, which improved its overall efficiency. Substantial improvements in performance were achieved by improving the supporting software and significantly restructuring the parallel codes.

The production phase

The system was in friendly user mode until it went into production in May 1993 [see *access*, Fall 1993]. Although scalable systems are totally different from traditional vector processing systems, the demand for access to NCSA's CM-5 system has been strong from the beginning.

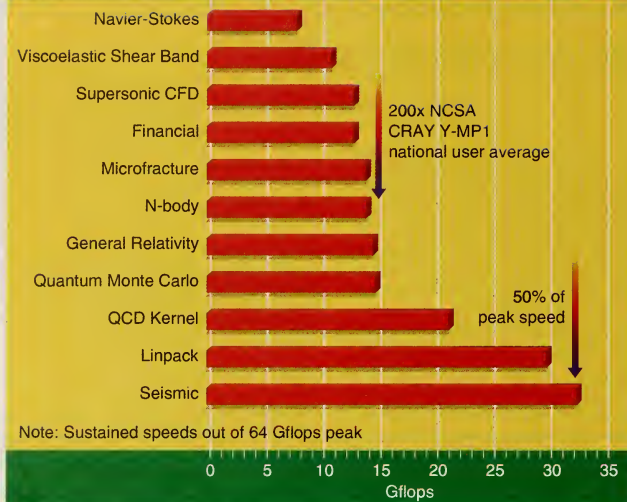
CM-5 users at NCSA constitute a broad range of researchers from Grand Challenge users at the high end to start-up users who want to test out scalable systems at the lower end. The number of active users on this system has grown steadily.

An analysis of the growth in usage of the CM-5 during the first six months since the vector units were functional at NCSA can be compared

Teraflop continued on page 6

This is a shortened version of an NCSA technical report “Marching to the Teraflop: The NCSA CM-5 in FY94.” The full report can be accessed online by following the directions on page 17.

NCSA's 512-node CM-5 Application Codes



Teraflop continued from page 5

and contrasted with the same time-frame after the introduction of traditional vector supercomputers in the past. The distribution of usage by project on the scalable system is very similar to the early days of traditional vector processing—both on the CRAY X-MP and the CRAY-2 systems. In fact, there are significantly more users running large jobs on the CM-5 than there were on the CRAY X-MP supercomputer during its first six months at NCSA!

Grand Challenge applications

So far, more than 140 projects have obtained peer-reviewed allocations on the CM-5. Twenty-three of these projects were allocated time on NCSA's CM-5 during the second year of the MetaCenter Grand Challenge Allocation program in March 1994. These Grand Challenge projects are from diverse disciplines including astronomy, chemical and thermal systems, materials research, molecular biology, and physics.

Six federally funded Grand Challenge research projects are described on pages 7 through 13. All are utilizing NCSA's CM-5. For a list of current MetaCenter Grand Challenge projects running on the CM-5, see page 17.

The distribution of projects by discipline on NCSA's CM-5 shows a broad interest in scalable systems across NSF scientific directorates. In contrast to earlier platforms at NCSA, one-third of the projects are computer science research projects. These projects have enabled and empowered researchers in other disciplines because their findings have provided advanced and optimized algorithms suited to scalable architecture. This response is quite different from the early Cray usage at NCSA when less than 1% of users were computer scientists.

NCSA's three-pronged approach—involving computational scientists, computer scientists, and Thinking Machines staff—helped identify and resolve bottlenecks with algorithms, compilers, and run-time libraries. As a result, the fastest CM-5 codes now achieve over 50% of peak speed. (See Figure 1.) Many users can now run 200 times faster on NCSA's CM-5 system than the national user aver-

CM-5 Utilization

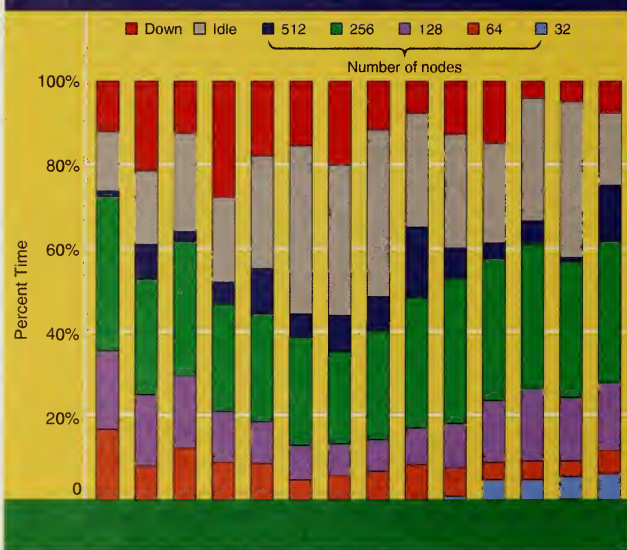


Figure 1 (above): Parallel Codes on NCSA's CM-5: Sustained Speeds out of 64 Gflops Peak.

Figure 2 (below): Utilization of NCSA's CM-5 by the National Research Community (Original graphs by Larry Smarr; technical illustration by Marshall Greenberg)

Teraflop continued on page 17

Simulations of quantum systems

by Thomas Krawczyk, Science Writer

Together with fellow UIUC Physics Professor Richard Martin and UIUC Computer Science Professor Roy Campbell, David Ceperley leads a 15-member group in the advancement of theoretical condensed matter physics.

The group has worked at solving the equations of quantum theory to build an understanding of atomic structure and find the properties of quantum systems at low temperature. They use NCSA's CM-5 to perform quantum mechanical simulations of electrons in solids (such as hydrogen at high pressure), of lattice models relevant to high-temperature superconductors, and of superfluid helium films.

This project has a grant from NSF's HPCC Computational Advances in Materials Research (CARM) Initiative and support from the Office of Naval Research.

QMC methodology

Quantum Monte Carlo (QMC) methods are the tools of choice—algorithms that use statistical sampling to solve the Schrödinger equation. Quantum mechanics accounts for the chemical and electronic properties of matter.

"The equations of quantum mechanics have been known since the 1920s," says Ceperley, an NCSA research scientist and leader of the Quantum Systems Group [see *access*, Spring 1993]. "To solve them is a very difficult—but purely a mathematical—problem. We would like the methods to be ultimately as accurate as a calculator is in adding two numbers. You trust it even if you never check it."

Supercomputing resources have helped further the group's research on hydrogen and helium. Although simple atoms, hydrogen and helium are also very complex in that their nuclei and electrons exhibit large quantum motion.

Studying helium

One focus of the group's work has been to describe the behavior of helium atoms at the transition temperature where helium changes from an ordinary fluid to a superfluid. This is particularly of interest to those in the field of superconductivity. Ceperley and Martin both are associate members in the UIUC Center for High-Temperature Superconductivity.

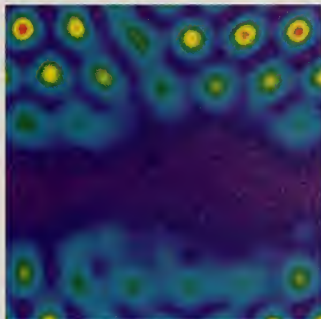
"There is a fundamental similarity between superfluidity and superconductivity. We would dearly like to do calculations on superconductors, but there is also a fundamental difference. Electrons are fermions and the simulation of fermions is much more difficult."

"In the past 10 years we have finally learned how to do really reliable calculations on bosons—liquid helium is the best example. Now we are starting to do the same for fermions, but it will take some time."

Advantages of the CM-5

Monte Carlo calculations are well suited to run on a scalable supercomputer by compiling the statistics from an arbitrary number of independent runs. An entire QMC calculation can fit on a single node, but accurate results require a long random walk.

Quantum continued on page 29



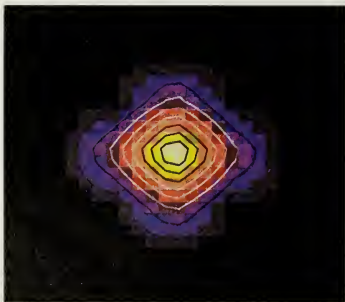
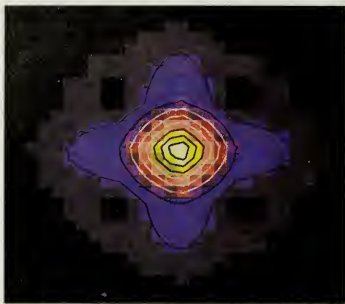
Density plot from path-integral Monte Carlo simulation of a bare solid H₂ (1,1,1)-surface with an incomplete top layer. Red represents high density and violet, low. Twenty-eight H₂ molecules in a simulated cell represent a half-filled layer showing a one layer high step in the surface. There are no H₂ molecules in the horizontal violet stripe. Some molecules ("washed out" chain) participate in quantum exchange; others display crystalline ordering. (Courtesy of David Ceperley and Marcus Wagner)



David Ceperley (Photo by Thompson-McClellan Photography)

Probing matter at its smallest scale with the CM-5

by Anne Simon Moffat, Science Writer



Images showing the distribution of quarks and antiquarks about a test charge in hadronic matter at high and low temperatures. Hadronic matter, a gas formed from strongly interacting elementary particles, undergoes a phase transition into a quark-gluon plasma at a temperature of about $T_C=200$ MeV. The quarks are liberated to wander freely at this phase. At low temperature ($T=75$ T_C) the number of quarks is large (above). At a higher temperature, thermal fluctuations screen the test charge and the system's response is smaller (below). (Courtesy Thomas A. DeGrand, MILC collaborator, University of Colorado, Boulder)

What is the basic stuff of the universe, the material from which everything is made?

For most of the first half of the twentieth century, scientists thought that protons, neutrons, and electrons were the most elementary particles. But, beginning in the 1950s, particle accelerator experiments revealed dozens of new, if short-lived, particles. So physicists gathered up their surprising data and proposed a revised order for the universe that said that the smallest bits of matter are quarks and leptons. These would then recombine into conventional protons or neutrons as well as the more bizarre, but fleeting, particles that were discovered in accelerator experiments. It was also proposed that in addition to the electromagnetic force, leptons interact by additional weak forces while quarks are bound by different, extremely strong forces that are carried by particles known as gluons.

The verification of the combined electroweak and strong forces theories has occupied particle experimentalists for the last two decades. The problem is that the interactions that bind quarks are so strong that, under ordinary conditions, individual quarks cannot be observed directly. Physicists have responded to this challenge by building higher energy particle accelerators that smash together either proton or electron beams—revealing important clues about the most basic forms of matter. The late physicist and Nobel Laureate Richard Feynman once described this experimental strategy as akin to learning how a pocket watch works by slamming two together and observing the debris fly out.

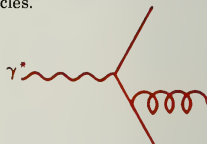
Scalable efficiency

The development of scalable supercomputers has offered a different strategy for probing matter on the smallest scale, an opportunity that is being seized upon by various groups of physicists. Researchers can now

use the most advanced computers, such as the Connection Machine (CM-5), to begin to study the interactions between quarks and gluons.

A widely distributed group of theoretical physicists, the MIMD Lattice Calculation (MILC) Collaboration is using NCSA's CM-5 to study how quarks and gluons behave at very high temperatures, such as those that existed in the early moments of the universe. The MILC Collaboration, a Department of Energy Grand Challenge applications group, includes Claude Bernard of Washington University in St. Louis, Thomas A. DeGrand of the University of Colorado in Boulder, Carleton DeTar of the University of Utah in Salt Lake City, Steven Gottlieb of Indiana University in Bloomington, Weiqiang (Charlie) C. Liu of the Thinking Machines Corporation in Cambridge, Robert Sugar of the University of California, Santa Barbara, and Doug Toussaint of the University of Arizona in Tucson.

"We want to learn about the basic building blocks of matter and the forces that hold them together," says Sugar. "We want to calculate the properties of strongly interacting particles, their masses, quantum numbers, and interactions with other particles."



Just as nineteenth century chemists used theory to organize the known elements into the periodic table with the hope that this master chart could lead to the discovery of new elements, modern physicists are trying to organize various combinations of quarks in a systematic way that might lead to discovery of new particles.

"We want to predict the masses of all possible combinations of particles

[made of quarks] and compare them with [available] experimental results," says Bernard. "There are big gaps in the evidence." There are also good signs that work on the CM-5 can help to fill those gaps.

Main challenges

One of the main challenges for these researchers is finding ways to deal with very large datasets. The theory that describes quarks and gluons is formulated in 4D space-time.

"There are many variables at every point in space and time," says Sugar, while adding that the large memory of the CM-5 makes it a particularly powerful tool for these studies.

Another challenge is presented by the fact that one of the physicist's most powerful tools for solving such complex problems, expansion in a small parameter, does not work here. In quantum chromodynamics, the theory of the strong interactions of quarks and gluons, there is no small parameter about which to expand. At present the only way to exact many of the predictions of the theory is through large-scale numerical simulations such as those in progress at NCSA.

"Nothing can be left out to simplify the problem," says Sugar. "We work with a small number of equations, but they are deceptive in that they are very difficult to solve." Bernard adds, "We cannot neglect trivial forces [in the computations] because nothing here is trivial. The only way to try and solve the problem is to use computer simulations." This is a task that is barely tractable, even for the most sophisticated computers; however, the strong floating point performance of the CM-5 provides the potential for making significant progress.

Varying temperatures

One favored simulation strategy is to study the change in properties of strongly interacting matter as the temperature is varied. The forces among quarks weaken as the temperature increases, and physicists believe that at sufficiently high temperatures they will find a new state of matter consisting of a plasma of quarks and gluons. The universe was presumably in this state prior to nucleosynthesis, and it may exist in the cores of neutron stars today. Nuclear physicists hope to observe

the plasma in heavy ion collisions in facilities such as the Relativistic Heavy Ion Collider now under construction at Brookhaven National Laboratory.

Throughout the world a number of theoretical physics groups are engaged in the numerical study of strongly interacting matter at high temperature. They have made a rough determination of the crossover temperature, which is approximately 1.7 trillion degrees Kelvin. Present indications are that the crossover between the low-temperature regime of ordinary matter and the high-temperature quark-gluon plasma is a smooth one, rather than a bona fide phase transition as in the boiling of water or magnetization of iron. A great deal has been learned about the properties of the plasma that are important for the interpretation of heavy ion collisions.

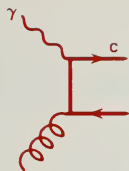
Looking ahead

Physicists have also begun to calculate detailed properties of the particles formed from different combinations of quarks both above and below the crossover temperature. For example, they are able to calculate the mass of various quark combinations in the low temperature regime to within 10 or 20% of experimental results. A future goal is to refine these calculations to make predictions of masses to 1% accuracy.

In its work at NCSA, the MILC Collaboration is creating a library of equilibrated lattices (snapshots of the system being studied) for use in its own work and for use by other physicists who are interested in related problems.

Sugar says that although the use of the CM-5 allows for significant advances, it represents only the beginning of what will be a new generation of computational studies of one of nature's fundamental theories.

"We are getting good performance on the [CM-5] machine," says Sugar, while noting that both its hardware and software are very new. "But we are only beginning to carve up what is a very large problem." ▲



Tools of the trade

By all accounts, numerical studies of the basic forces and entities of matter require enormous computational resources. The CM-5 provides an important new tool for this work.

The numerical studies are carried out within a framework called lattice gauge theory (LGT), a mathematical scheme developed almost 20 years ago for discretizing problems involving quarks and gluons. Discretization is essential if one is to carry out numerical studies.

First formulated by physics Nobel Laureate Kenneth Wilson of Ohio State University, LGT sets the stage for describing quark-gluon interactions by putting them on a 4D lattice (three Cartesian coordinates and a fourth for time), on which quarks hop from one lattice point to another interacting with forces carried by gluons.

Although a variety of computers have been used to perform LGT calculations for a decade or more, the arrival of the CM-5 and other large scalable computers offers a new opportunity. Their memory and computational power are so great that they allow calculations to be carried out on significantly finer lattices than has previously been possible. In turn, this greatly improves lattice gauge theorists' ability to extract accurate physical results from their simulations.

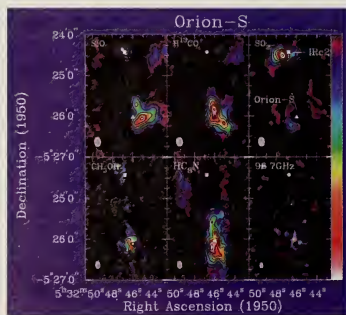
"We have experimented with and written code for a wide variety of parallel machines—the nCUBE 64000, Intel's iPSC-860 and Paragon, and the CM-2," says Sugar. But the CM-5, he adds, "offers the most powerful and stable computer resource at the time."

The team's program runs on 128 or 256 of the machine's 512 nodes, with 90% of the computer effort running at 40 Mflops per node, an extraordinarily fast rate of computation that Sugar credits to the efforts of Applications Engineer Charlie Liu, a Thinking Machines representative who worked onsite at NCSA until recently.

Feynman diagrams adapted from *Quarks & Leptons: An Introductory Course in Modern Particle Physics* by Halzen and Martin (1984).

Radio synthesis imaging

by Thomas Krawczyk, Science Writer



Molecular clouds in Orion, imaged with the BIMA array. (Courtesy of Richard Crutcher)

Orion



Richard Crutcher (Photo by Thompson-McClellan Photography)

Radio telescope synthesis arrays are usually located far from the astronomers who need the data. In addition, the astronomical data collected from separate radio antennae all focused on a single source are not an image until run through a Fourier Fast Transform (FFT) via computer. Insufficient computing resources have made some cutting-edge research virtually impossible.

UIUC Astronomy Professor Richard Crutcher's goal is to remove the computing bottleneck by creating the next-generation radio telescope imaging system. With a high-speed communications network in place, researchers could actively control a remote radio telescope array, route the data through a metacenter computing environment, and display the resulting images on graphics workstations in their own offices.

Other collaborators on this project, which is funded by NSF, include Leo Blitz, Charles Catlett, E. Churchwell, Michael Heath, Linda Sparke, Mark Stupar, Bart Wakker, and W. J. Welch.

Refining the system

Parts of this system are already in place. Crutcher gathers data in northern California from the millimeter-wave Berkeley-Illinois-Maryland Association (BIMA) Hat Creek Observatory. The data are then sent over NSFNET to NCSA's distributed computing environment, which provides the necessary imaging engine. The most computationally intensive routines will be run on the CM-5, with the rest of the code running on the CONVEX C3880 or SGI Onyx, which is linked to the CM-5 via HIPPI.

Results can be displayed in 3D color on a Silicon Graphics workstation. Plans are now underway to demonstrate remote control of the operation from the University of

Wisconsin at Madison over the BLANCA gigabit/second testbed network [see *access*, Fall 1993].

If a simple FFT of the data were the only computational requirement, a modest computing system might suffice. Radio telescope synthesis arrays, however, suffer from two factors that greatly degrade the image. First, a radio telescope's own instrumental signature corrupts the data received from the astronomical source. Much like an optical telescope's addition of diffraction rings to the image of a point source, a radio telescope has a "point spread function" that interferes with the true source signal. Second, instrumental and atmospheric instabilities add to random fluctuations that contaminate the signal.

Avoiding "dirty" signals

Two techniques can overcome a great deal of the noise associated with a "dirty" signal. Deconvolution is used to reverse the blending of the instrument signal with that of the source. In the optical telescope example, the diffraction rings could similarly be removed from the image itself. There are several methods to achieve deconvolution, but all are intensely iterative.

Similarly, self-calibration is the method of comparing a telescope's data with that of the other telescopes in an array. For example, the 27 telescopes of the Very Large Array in New Mexico can be connected in every combination so that 351 signals are available. Astronomers can then use 27 of the signals to calibrate the telescopes and the remaining 324 for imaging of the radio source. Again, the iterative process is computationally intensive.

Radio synthesis continued on page 29

Biomolecular modeling and structure determination

by Thomas Krawczyk, Science Writer

BIOLOGICAL SYSTEMS

UIUC Physicist Klaus Schulten and his interdisciplinary Theoretical Biophysics Group seek to improve modeling and structure determination calculations in molecular biology. The group employs scalable computers, such as NCSA's CM-5, to solve problems that are impossible to determine otherwise.

"Our goal is to use the new generation of parallel computers as a research instrument in molecular biology," says Schulten. "We will develop algorithms that will be suitable for these computers. However, we cannot just rely on the power of the new computers, but need to also develop faster algorithms."

Once the codes are ready, the group will shift to another of their Grand Challenge goals. "We want to be sure that the fruits of this labor become available to a broad group of biological scientists," Schulten says. Schulten plans to collaborate with Yale Biophysicist Axel Brünger to incorporate his algorithms into Brünger's version of the well-known structure refinement and modeling program called X-PLOR.

Broadening opportunities for biologists

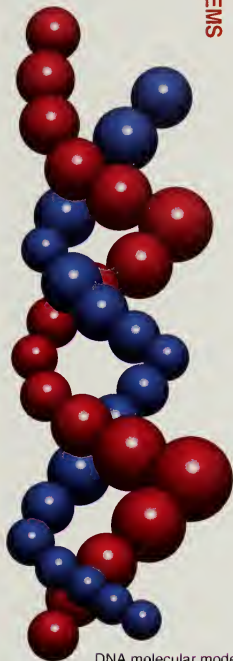
X-PLOR is currently one of the most widely used programs in computational biology. Schulten feels that

upgrading X-PLOR would "make certain that not just a small, elite group of people with extreme research problems in mind has an advantage, but that their efforts also trickle down to the broad community of computational biologists."

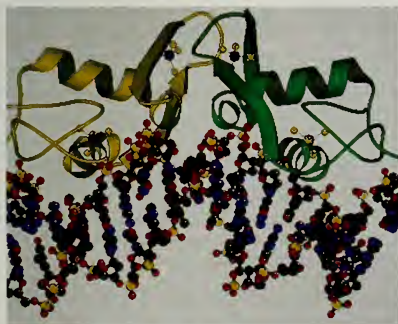
Dissemination of information has always proven difficult, even among the principal investigators themselves. "We have a group of researchers at five different sites," says Schulten, "and that creates logistics problems. We feel we have to work very tightly together and basically form one group. We will use workstation-based teleconferencing to allow students and postdocs at different sites to share monitor images and discuss their research." Schulten's group has also used NCSA Mosaic and Collage software tools to help bridge the communication gap.

Enhancing communication

Another problem involves building a viable seminar program. Organizing seminars is difficult due to the nature of the field—the university departments are either computing oriented or biology oriented. "This is a small field," says Schulten. "We will organize seminars that emphasize both structural biology and computing. We intend to broadcast the seminars first among the participating groups and later to other interested sites." Once



DNA molecular model with double helix (Illustration by Linda Jackson)



Biomolecular continued on page 28

Complex of two glucocorticoid receptor proteins (top) with DNA (bottom). Molecular dynamics simulations carried out on a 64-processor scalable computer indicate that the two proteins bend the DNA downward. (Courtesy of Klaus Schulten and Tom Bishop)



Klaus Schulten (Photo by Thompson-McClellan Photography)

Astrophysical crash: Comput

Scientists at The University of Texas at Austin, NCSA/UIUC, and six other universities are collaborating on a Grand Challenge effort to investigate what happens when two black holes collide.

NSF's High Performance Computing and Communications Program awarded \$3.75 million—\$550,000 for NCSA input—to fund the research.

"It's a big project to try and compute," says Ed Seidel, NCSA research scientist and leader of its Relativity Group. "It's a step-by-step process. Each time we add a step there will be a whole new set of problems to solve."

The project will start simply, with the simulation of two nonspinning black holes colliding head-on. Next, spins aligned along the collision axis will be modeled. Finally, the simulation will include the black holes spinning and revolving around each other and colliding.

Principal investigator is Richard Matzner of the Center for Relativity at The University of Texas at Austin. Other co-principal investigators are James Browne (University of Texas, Austin); Larry Smarr and Ed Seidel (NCSA/UIUC); Paul Saylor and Faissal Saied (UIUC); James York and Charles Evans (University of North Carolina, Chapel Hill); Stuart Shapiro and Saul Teukolsky (Cornell University); Geoffrey Fox (Syracuse University); Jeffrey Winicour (University of Pittsburgh); Sam Finn (Northwestern University); and Pablo Laguna (Pennsylvania State University). Each group is contributing their own unique talents and insights. In this article we review only one piece of the NCSA/UIUC effort.

Solving Einstein's theory

Scientists will use the black hole simulation to find out more about data they may be receiving from the Laser Interference Gravitational Wave Observatories (LIGO), which will be working by the year 2000. These highly sensitive devices will detect

tiny disturbances in the gravitational field produced by cosmic sources, such as colliding black holes.

"We are solving Einstein's equation for the collision of black holes so we can understand LIGO's data and differentiate black hole collisions from other astrophysical events," says Karen Camarda, UIUC graduate research assistant working with Seidel.

Einstein found that gravity is a property of space-time, not just a force. He predicted that gravitational waves would ripple through space in the same way that waves ripple through a pond. His equations of General Relativity govern these time-changing curvatures.

"After almost 80 years, it is time for us to start solving these equations, and the only way we know how is through supercomputers," Seidel says. "The equations are so complicated that is beyond our capability to find a general analytic solution. Einstein sat down with very basic theories and figured it all out—that's the amazing thing."

Opening the door

According to Seidel, solving these equations will "open the door" to studying the physics of gravity.

"There will be much to do," he says. "One thing will be comparing the precise predictions of Einstein's equations to experimental and observational results that will be available during the early part of the next century. Such comparisons should point the way towards future research.

"For example, one may find that experiments do not agree completely with the theory. If the calculations can be trusted, one would have to consider modifying Einstein's theory. So we will be able to verify the theory in precise detail, and perhaps we will find that it is inadequate in some ways—although so far every indication is that it is the correct theory of gravity."

Evolution of a distorted black hole system.

Black line shows the black hole's horizon.

(Courtesy Ed Seidel, Peter Anninos, David Bernstein, David Hobill, Larry Smarr, and John Towns, science; Mark Bajuk, visualization. Stills from NCSA visualization archives)

ting colliding black holes

by Victor Ryckaert, Student Writer

If Einstein were still alive, Seidel says, "I think he would like it."

Using multigrids

Being a Grand Challenge project, researchers from many disciplines are helping to work out the Einstein equations. UIUC computer scientists Associate Professor Faisal Saied and Professor Paul Saylor are developing better ways to streamline computing resources for this extremely complex problem.

For the most part, scientists will be solving hyperbolic equations, which run efficiently on scalar machines like NCSA's CM-5. Bottlenecks occur when computing the partial differential equations needed for solving elliptical problems.

Typical methods deal with all scales on a fine grid which wastes resources. Multigrid methods cheaply eliminate the high-frequency error components on the fine grid and deal with lower frequency errors on coarser grids where they are more easily handled. Such methods are "optimal order," meaning that the cost of finding an unknown value remains fixed as the problem size increases—with other methods, the cost increases more rapidly.

Refining the method

Saied and Saylor are working towards adapting a more effective multigrid approach. "Multigrid methods derive their efficiency from separating out different spatial or length-scales by using a sequence of nested grids," says Saied.

Scientists say the numerical solution can drift from the true solution due to numerical error. "Multigrid is the engine making the car go down a curved road. We are the navigation constraining the car to the road," says Saylor. He describes the curved road as an elliptical problem and notes that it is his and Saied's task to make the computations run smoothly.

"An important challenge for current research is to come up with effective parallelizations of multigrid methods on distributed memory parallel machines," Saied says. "The difficulties stem from the global data dependencies, and hence global communication requirements, of elliptical problems."

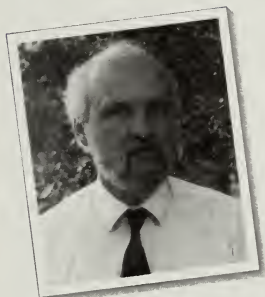
Saylor and Saied note that their work is still in the early stages. "We've done 1D equations and are bridging the gap to 3D," Saylor says.

Others working on the project at NCSA include Director Larry Smarr, co-principal investigator; postdoctoral research associates Peter Anninos and Joan Masso; graduate research assistants Steve Brandt, Joe Libson, Peter Leppik, Bharat Khardia, and Paul Walker; and research programmer John Towns.

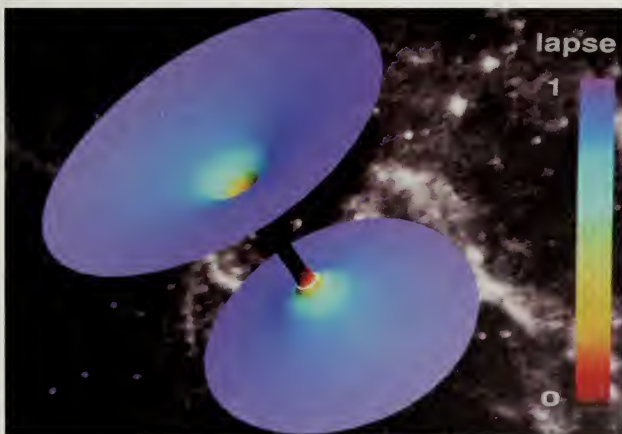
This project will exploit scalable computing to develop software tools using NCSA's CM-5 and the Pittsburgh Supercomputing Center's T3D system.

Further information

To find out more about NCSA's Relativity Group, including their research reports and project descriptions, see their Home Page via NCSA Mosaic. The URL is: <http://jean-luc.ncsa.uiuc.edu/> ▲



Richard Matzner



Numerical relativity: black hole space-times. Embedding diagram describes the behavior of the gravitational field for a single black hole. Color shows speed at which idealized clocks measure time—blue, slow; red, fast. (Courtesy Larry Smarr, David Hobill, and David Bernstein, science; Donna Cox, visualization)

The algorithms are here by Victor Ryckaert, Student Writer

It is easier today for astrophysicists to use state-of-the-art algorithms thanks to the efforts of NCSA scientists and funding from NSF.

NSF's Astronomical Instrumentation and New Technologies program awarded \$250,000 over two years to NCSA's Laboratory for Computational Astrophysics on May 1, 1993. The LCA [see *access*, May-June 1992] provides access to community codes via electronic mail, NCSA Mosaic, and the Andrew File System.

"We want to be a clearing house for theoretical astrophysics software in addition to developing our own," says LCA director Mike Norman. "We are trailblazing by developing and providing community codes. They are unknown for astrophysics."

"Astronomy has been slowed down because codes are only in the hands of the people who know how to use them," says Dimitri Mihalas, NCSA principal investigator and UIUC astronomy professor collaborating with Norman.

Codes out in early 1994

The LCA released three codes at the January meeting of the American Astronomical Society—ZEUS-2D, ZEUS-3D, and TITAN, says Norman, NCSA research scientist and UIUC astronomy professor.

"It is such an effort to get the latest codes, at some time you just want to build on them," postdoctoral research associate Michael Gehmeyr says.

"It's not that people do not want to use these codes," says Mihalas, creator of TITAN. "They have other expertise and want a reliable tool. Scientists want to take the computer's results and work with them. When we turn our TV set on, we do not necessarily want to know how it works, we just want to watch. Not every astronomer who uses a telescope knows how to build one."

ZEUS-2D and ZEUS-3D codes

ZEUS-2D and ZEUS-3D are both time-explicit astrophysical fluid dynamics codes. Both versions can be used to simulate astrophysical fluid flows, including the effects of magnetic fields and self-gravity. ZEUS-2D adds radiation hydrodynamics, the interaction of light and matter, into the equations.

Norman says that ZEUS-2D is a proving ground. "Scientists use it to build physical intuition before attacking a problem in 3D."

Modeling the universe

The NCSA Astrophysics Group's area of study is the entire universe—ranging in scale from its history and formation to the properties of individual structures within it. With Princeton University's Jeremiah Ostriker and other collaborators from across the country (see names below), they are tackling problems on a wide range of length-scales, including the structure of supersonic jets and cosmology.

The multiscale nature of these problems, as well as their nonlinear character, classify them as Grand Challenges. Group Leader Mike Norman states the group's goal as "setting the benchmark of excellence in these disciplines."

Supersonic jets

Astrophysical jets are supersonic streams of material ejected from the centers of active galaxies and star-forming regions.

"No one has ever simulated a supersonic jet in 3D with enough resolution to address simple questions," says Norman, a UIUC professor of astronomy and NCSA research scientist. Among such questions are: "What is the structure?" "How stable is it?" "How far can it propagate before it falls apart due to instability?"

To study these phenomena, Norman, Greg Bryan, graduate student in astronomy; and Jim Stone, former postdoctoral research associate, have employed the CMHOG (Connection Machine Higher-Order Godunov) code on NCSA's 512-node CM-5. CMHOG implements the PPM (piecewise parabolic method) algorithm, developed by Paul Woodward at the Army High Performance Computing Research Center.

"CMHOG is the fastest implementation of the best algorithm on one of the largest parallel supercomputers in the world," Norman says. "It is like a big hammer. What do you do with a hammer? You go around squashing things. We are going to beat on a lot of classical problems."

The NCSA team's most recent jet calculation contained 32.5 million zones and ran at 12.5 Gflops on the CM-5. A striking visualization of this jet appears much like fire.

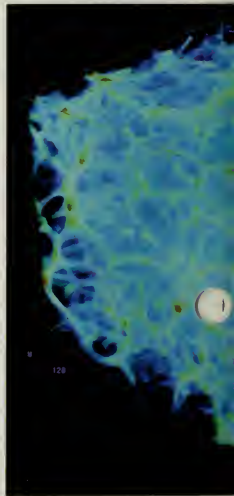
Immediate plans are to run a 100 million-zone calculation. Bryan says this large calculation will allow the group to probe why a jet seems stable for great distances and then suddenly stops.

"This phenomenon has a lot to do with turbulence," Bryan says. "The key thing is that it works on many scales. We want to resolve as many of those as possible."

Cosmology

Cosmology is the study of the content and evolution of the universe. The Astrophysics Group recently simulated the universe's large-scale structure in 2D using a version of CMHOG, "which describes how the primordial gas clusters under its own gravity," Bryan says. This code is called KRONOS, after Greek mythology's father of time. KRONOS, which also runs on the CM-5, incorporates CMHOG and an N-body code for evolving the dark matter.

A visualization of this simulation (right) shows the large-scale structure as intersecting filaments. These filaments represent sheets of galaxies that are typically 100 million light-years from end to end. The in-



verse on the CM-5

by Jarrett Cohen, Staff Associate, Director's Office

tersections are clusters of galaxies, ranging in length from 1 to 10 million light-years. Galaxies are typically less than 100,000 light-years in diameter.

NSF is funding further work in this area through a five-year HPCC Program Grand Challenge grant of \$3.2 million; NCSA will receive approximately \$650,000 of the grant.

The principal investigator is Princeton University's Jeremiah Ostriker, with whom Norman has collaborated for several years [see *access*, September–December 1991]. The other researchers in the Grand Challenge Cosmology Consortium (GC³) are David Spergel (Princeton University), Ralph Roskies (Pittsburgh Supercomputing Center), Dennis Gannon (Indiana University), Daniel Reed (UIUC), Edmund Bertschinger (MIT), and Lars Hernquist (University of California, Santa Cruz).

The consortium is going to use NCSA's CM-5 to simulate the formation of galaxy clusters and compare them with real clusters in the universe. These clusters are represented by the red regions in the filament visualization shown below.

A multiscale algorithm

Doing numerical cosmology properly involves simulations on multiple scales, Norman says. "Throughout the history of computational physics, researchers have worked at the single scale. They pick a domain and stay within it, disregarding what is happening outside of it."

"One can do that if what is going on outside has very little influence. Unfortunately, that is not the case if gravity is the prime influence, which it is in this field," he says. "These structures are entirely the result of gravity operating on initially small density fluctuations and [then] amplifying them."

From the galaxy sheets to a single galaxy is a factor of 1,000 in length-scale, or 3 orders of magnitude. "Our goal is to resolve the process of galaxy formation. You need at least a grid fine enough to put 10 zones across a galaxy—a grid resolution of 10,000 light-years," Norman says.

There are two possible approaches to simulating this multiscale problem at the needed resolution. One is what Norman calls the "brute force" method, running a simulation with 10,000 zones on a side. "This is feasible in 2D using current computers, but out of the question in 3D."

He imagines doing an $10,000^2$ simulation and getting resolution of 100 million zones but says it is not now possible to consider all the scales at 10^{12} , which is

Universe continued on page 16

3D visualization of the large-scale structure of the universe. Intersecting filaments represent sheets of galaxies; intersections indicate clusters of galaxies. (Courtesy Mike Norman)

ZEUS-3D provides the geometrical complexity of the real world. To get the realistic view, however, the code sacrifices the physical complexity of radiation hydrodynamics.

Both ZEUS codes are used for investigating supernova explosions and astrophysical jets. Being time-explicit, they can only look at relatively short time-steps (the time it takes a sound wave to cross a computational cell) because the solution of a given step is based on the results of the data from the step before.

TITAN code

This is where TITAN fills the void. TITAN is a 1D, adaptive mesh radiation hydrodynamics code that is excellent for solving the stellar hydrodynamics of the inside of a star, for example stellar pulsations. Being time-implicit, TITAN can investigate much larger time-steps because it uses the future solution to solve itself. This allows the simulation of slow, evolutionary processes as well as quick dynamic events.

ZEUS-2D and ZEUS-3D are designed to run on any conventional vector supercomputer or a superscalar multiprocessor system. They can run on high-performance workstations for small problems. TITAN runs on vector and superscalar uniprocessor machines.

There are currently 42 registered LCA users at 28 institutions in three countries.

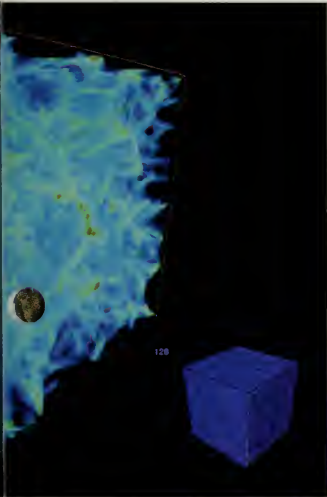
For more information

To find out more about the LCA, check out the Home Page using NCSA Mosaic at URL: http://zeus.ncsa.uiuc.edu:8080/lca_home_page.html.

ZEUS and TITAN documentation are available via anonymous FTP. For more information, contact Robert Fiedler at rfiedler@ncsa.uiuc.edu (Internet).



Jeremiah Ostriker
(Photo by Jodi Levinson)



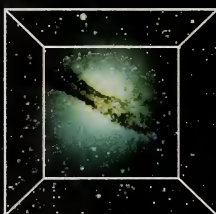
Multiscale Numerical Cosmology and Galaxy Formation

Gas dynamics
+ stellar dynamics

Galaxy Scale ($d \leq 100$ kpc)

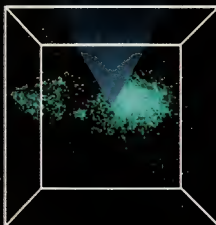
Dark matter
+ gravity
+ gas dynamics
+ stellar dynamics
+ radiation

1



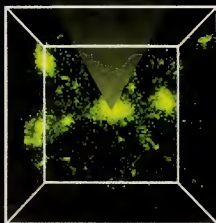
Cluster
Scale

2



Supercluster
Scale

3



Large Scale
($d \leq 100$ Mpc/h)

4



Dark matter
+ gravity

Universe continued from page 15

(10^4)³, or the factor difference between the large-scale universe and single galaxy grids cubed.

A much more intelligent approach, says Norman, is refining locally using a multiscale algorithm. An interdisciplinary project called HAMR (Hierarchical Adaptive Mesh Refinement) is the key here.

"Using HAMR, we will be able to achieve effective resolution of $10,000^3$, which is what we need to do the galaxy formation problem," Norman says. "We hadn't had a big enough computer to solve a multiscale algorithm. HAMR [on the CM-5] will crack this open."

HAMR

HAMR is a general-purpose system being developed by Henry Neeman for his Ph.D. dissertation in computer science at UIUC. It is a library of subroutines and functions written in C. When completed, it will allow the construction of any hierarchical grid application.

Norman says HAMR is "like a Russian doll—a doll within a doll within a doll." However, "if you had HAMR, you would still have quite a bit of development remaining to have a cosmology or combustion code," he adds. "Our plan is to take HAMR and build a cosmology code—NC Hammer." NC stands for Numerical Cosmology.

The basic idea of HAMR is to use coarse zones where possible, only refining grid resolution where needed. Norman says one starts a simulation on a coarse grid. "As structure develops, the system has built into it various thresholds . . . that refine the grid locally. The key word is *locally*. We are trying to get away from refining the whole grid to the desired resolution."

HAMR will introduce finer subgrids in necessary places. "There is no restriction on the number of subgrids or levels of refinement," Norman adds.

Norman compares the grid hierarchy to UNIX directories. The large scale is the root directory, or base grid. A simulation is begun on this base grid at a low resolution, perhaps 64^3 or 128^3 . "Then the simulation proceeds, and structures develop. Level 1 subgrids are introduced, centered around regions where structure has developed.

"If those structures are adequately resolved by the subgrids, stop," he says. "But usually a cascade of structures form within the subgrid, and they need further refinement—level 2 subgrids."

At the higher level subgrids, Norman explains that they can use the same number of zones but get a higher resolution because of the smaller size of the "box" they are considering.

In one possible example, Norman imagines starting with a 64^3 calculation, which would give birth to a bunch of 64^3 calculations. "At the end, you may have over 100

Universe continued on page 28

Diagram of the GC³ Multiscale Numerical Cosmology Scheme.

Note: View 4 is four orders of magnitude greater than view 1.

(Data from Mike Norman; technical illustration by Marshall Greenberg)

age on our CRAY Y-MP system's single processors.

In addition to speed, NCSA's CM-5 allows users to study much more complex problems by offering a total of 16 Gbytes of memory. Large-scale applications codes written by computational scientists have already effectively made use of this large address space. In contrast, the largest job they can run on the CRAY Y-MP system today is 256 Mbytes.

The use of our CM-5 by the national research community continues to grow. (See Figure 2, page 6.) In February 1994, the machine was idle less than 20% of the month. The utilization of the parallel partitions reached 96% for the largest 512-node partition.

The age of scalable computing has begun. Success stories are coming in so fast that print media must be supplemented to keep NCSA's users abreast of breaking developments. For this reason, a CM-5 User Group has begun. Called the International Connection Machine User Group (ICMUG) it utilizes NCSA Mosaic to bring together CM-5 sites worldwide. To obtain current information about the ICMUG, follow the directions on the inside back cover for accessing the NCSA Home Page.

Online report

A complete, more detailed version of this report is available from the NCSA Home Page under the technical reports, reprints, and preprints section. For directions on how to obtain the full report from Gopher

or anonymous FTP, see the inside back cover. Abstracts of Grand and National Challenge projects are included in the complete report.

NCSA is positioned to enable researchers operating in the computational vanguard of their disciplines to accomplish their goals. Both academic (engineering, fluid dynamics, materials sciences, etc.) and industrial (seismic, financial) codes are achieving high speeds as demonstrated by the examples of research in the online version of this report. Significantly these large-scale projects—all utilizing the refined CM-5—encompass Grand Challenges and National Challenges. ▲

1994 MetaCenter allocations (formerly MetaCenter Grand Challenge allocations)

Awards for MetaCenter research allocations granted by the MetaCenter Allocations Committee (MAC) were announced in March 1994. Those utilizing NCSA's CM-5 and CONVEX C3 follow. The amount of time is stated in Service Units.

Edmund Bertschinger, MIT, "The Formation of Galaxies and Large-Scale Structure," 10,000 SUs [CM-5]; 17,400 SUs [C3] (block grant).

David Ceperley, UIUC/NCSA, "Simulations of Quantum Systems," 3,450 [CM-5]; 700 [C3].

Marvin Cohen, Univ. of California, Berkeley, "Theoretical Solid State Physics," 4,740 [C3].

William Goddard, CalTech, "Atomistic Simulation of Biological, Chemical, and Materials Systems," 1,000 [C3].

Keith Gubbins and Athanassios Panagiotopoulos, Cornell Univ., "Molecular Simulation of Fluid Behavior in Narrow Pores and Pore Networks," 4,000 [CM-5].

Herbert Hamber, Univ. of California, Irvine, "Studies of Quantized Gravity," 2,000 [CM-5].

John Joannopoulos, MIT, "Ab Initio Simulations of Materials Properties," 3,600 [CM-5].

George Karniadakis, Princeton Univ., "Unstructured Spectral Elements: Parallel Simulations of Turbulence and Microtransport in Complex Geometries," 2,000 [CM-5].

Gregory Kilcup, Ohio State Univ., "Investigation of Spectrum, Decay, Constants, Bk, and Semileptonic Form Factors in Lattice QCD with Wilson Fermions," 5,000 [CM-5].

Ronald Levy, Rutgers Univ., "Supercomputer Simulations of Liquids and Proteins," 3,000 [CM-5].

Richard Matzner, Univ. of Texas, Austin, "Black Hole Binaries: Coalescence and Gravitational Radiation," 625 [CM-5].

James McCammon, Univ. of Houston, "Theory of Biomolecular Structure and Dynamics," 3,000 [C3].

Russ Miller, SUNY, Buffalo, "SnB: Crystal Structure Determination via Shake-and-Bake," 3,500 [CM-5].

Klaus Schulten, UIUC, "Simulations of Supramolecular Biological Structures," 3,000 [CM-5].

H. Edward Seidel, UIUC/NCSA, "Computational Relativity," 10,000 [CM-5]; 125 [C3].

Shankar Subramaniam, UIUC/NCSA, "Computer Simulation of Molecular Recognition in Proteins," 2,000 [C3].

Robert Sugar, Univ. of California, Santa Barbara, "Lattice Gauge Theory on MIMD Parallel Computers," 9,700 [CM-5].

1994 allocations continued on page 18



1994 allocations continued from page 17

Norman Wagner, Univ. of Delaware, "Massively Parallel Simulations of Colloid Suspension Rheology," 2,000 [CM-5].

Robert Wilhelmson, UIUC/NCSA, and **Louis Wicker**, Texas A & M Univ., "The Numerical Simulation of Convective Phenomena," 1,700 [CM-5]; 600 [C3].

Bernard Zeigler, Univ. of Arizona, "Massively Parallel Simulation of Large-Scale, High-Resolution Ecosystem Models," 4,000 [CM-5].

The MetaCenter Allocations Program assists researchers in utilizing distributed heterogeneous computing across multiple centers. The program is aimed at projects that are computationally massive, resource intensive, or interdisciplinary. Proposals for allocations on the high-performance machines of the MetaCenter are accepted once yearly by the MetaCenter Allocations Committee.

The 1994 MetaCenter Allocations Program (renamed from "Grand Challenge" to avoid confusion with NSF's Grand Challenge Program) that provided allocations across all NSF supercomputing centers was coordinated by the Pittsburgh Supercomputing Center, 4400 Fifth Avenue, Pittsburgh, PA 15213-2683; (412) 268-7143.

For details about how to apply for time on NCSA's high-performance computing systems, contact Allocations [see **nCSA contacts**, page 2]. ▲



NCSA's Machine Room (June 1993). Forming part of NCSA's metacomputer, the machines are (left to right) Connection Machine Model 5 (CM-5), Hewlett-Packard PA-RISC 735 cluster, CONVEX C3880 (C3), and CONVEX C220 (used for mass storage). (© David Parker/Science Photo Library, 1993)

SCHLUMBERGER: FAST, SCALABLE SEISMIC PROCESSING

NOTE: Schlumberger, one of NCSA's newest industrial partners, has employed large-scale parallel computers in commercial seismic processing since 1991, when a service using a Connection Machine Model 2 (CM-2) was introduced. Today, Geco-Prakla (Schlumberger's seismic company) offers several advanced services on Connection Machine Model 5s (CM-5s). The following report is adapted from "Production 3D One Pass Seismic Migration on the Connection Machine 5" by Peter Highnam, Andy Pieprzak, and Jeff Rutledge of Schlumberger with permission.

Seismic exploration is a crucial early step in oil exploration. Data are acquired from surface surveys, processed, and interpreted in order to understand the subsurface structure of a region. The duration of the processing for a 3D seismic survey can be measured in months, and datasets of over a terabyte are not uncommon. A sequence of processing steps are applied to the acquired data. The earlier steps are concerned with (1) ensuring that the acquisition location and data are correctly registered and (2) improving the signal content. After these steps have been completed, the original data volume is typically reduced by a factor of 60 or so. The next step is to apply an imaging process called seismic migration.

Migration accounts for a large proportion of the time spent in a typical processing sequence. The migration process combines acquired data with a proposed structural model and delivers a result volume in which seismic reflectors are placed according to the model and their record in the input data. There are many flavors of 3D migration. Highnam, Pieprzak, and Rutledge adopted one of the most accurate and computationally intensive migration processes: 3D one pass post-stack migration

using Hale's method [1]. Migration inputs and outputs are shown in the diagram below.

With the introduction of the CM-2 based migration service [2] in May 1991, Schlumberger became able to provide new levels of accuracy for the migration process without increased runtime, compared to traditional vector systems.

The CM-2 implementation sustains over 6 Gigafllops (Gflops) on a system with 2,048 floating point units. The same algorithm is available on the CM-5, where over 32 Gflops are sustained on a 512-node system.

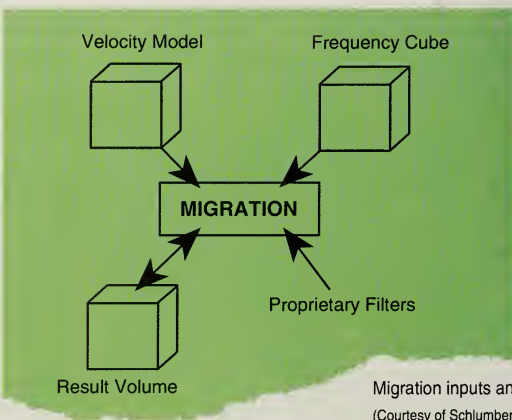
Timing measurements were performed on two CM-5s: a 128-node Schlumberger system and a 512-node system at NCSA. A CM-5 system can be partitioned into smaller groups of nodes. The team used this capability to time runs on 64-node, 128-node, 256-node, and 512-node partitions. All timings were made using "wall-clock" timers and include the time spent to move terabytes to and from the CM-5 disk subsystem. The team used problem sizes and parameters

that are representative of their commercial processing workload. Their results indicate that the code scales well with machine size. They demonstrated that the code can sustain around 50% or better of peak performance across the range of system sizes tested. Actual performance numbers ranged from 4.24 Gflops on a 64-node CM-5 to 32.67 Gflops on a 512-node CM-5.

For more information about this project, contact Peter Highnam by email at highnam@austin.slcs.slb.com (Internet).

References

- [1] Hale, D., 1990, "Stable Explicit Depth Extrapolation of Seismic Wavefields," 60th Annual International Meeting and Exposition of the Society of Exploration Geophysicists, 1301-1304.
- [2] Highnam, P. T., and Pieprzak, A., 1991, "Implementation of a Fast, Accurate 3D Migration on a Massively Parallel Computer," 61st Annual International Meeting and Exposition of the Society of Exploration Geophysicists, 338-340. ▲



Migration inputs and outputs.
(Courtesy of Schlumberger)

THE BRIDGES OF HPCC COUNTY

ILLUSTRATION BY JOHN HAVLIK

A long-standing goal of NCSA's Education Group has been encouraging teachers to "bridge the gap" between classroom science and the kinds of scientific research done by professional mathematicians and scientists—especially those using HPCC. A growing collection of postcards depicting bridges around the world hangs in the group's hallway to reinforce the goal.

Aware that students understand the value of science better when they see real-life applications of the con-

cepts they are learning, the group is bringing this idea into reality with its development of a variety of interactive simulations.

Building a Research-based Interactive Discovery Gallery for Education: The BRIDGE Project

Under the informal code name of the BRIDGE Project, the Education Group is developing materials to take advantage of the computing resources now available on Internet and training teachers to use them. It is also encouraging teachers to develop their own materials. As a result, teachers gain the proficiency to integrate what they have learned into their curricula, thereby exposing their students to real science. Students begin to do

science as scientists do science: making careful observations, thinking about the observations, studying what others have done, and asking "what if" questions that can only be answered by going back and making more observations.

Many simulation programs that run on personal computers usually available in the K-12 classroom permit students to examine interesting concepts, but their results only roughly and symbolically approach reality. The speed of the classroom computer forces approximations to be introduced that speed up the programs so they run in less than a class period. In contrast, the interactive simulation programs developed at NCSA harness HPCC technologies to offer higher fidelity or closer approximations of reality. These simulations have been adapted from simulations used by scientists working at or with NCSA and its resources. In some cases, they are the *same* simulation codes. Students then use real scientists' tools to generate, gather, visualize, and analyze real data. Not only does this allow students to study exciting questions never before possible in a K-12 classroom, but students are able to ask and help to answer questions that intrigue today's scientists.

Several NCSA scientists and UIUC graduate students, besides helping with the development of these simulations, have made themselves available as network mentors so that student users can "ask the experts" as questions arise. Members of the Education



Bridges continued on page 22

Group are also scanning the network to keep up with developments at other centers, identifying a variety of applications that can now be brought into the K-12 classroom. Several of the simulation programs developed and utilized by NCSA's Education Program are described below.

ChemViz is a tools and materials development project that enables advanced chemistry topics to be addressed in the high school curriculum by harnessing HPCC technologies [see *access*, July–September 1992]. This project typifies the approach to Client-Server Science, the heart of the BRIDGE Project. In this approach:

1. the *client* is an easy-to-use Macintosh application that sets up or controls calculations,
2. the *server* is a remote supercomputer accessed by modem or Internet, and
3. the *science* is represented by the fact that the codes running on the supercomputer and the techniques used to visualize the data are the same as those used by research scientists studying the same topics.

With Chem Viz, the user runs the program **Boogie** on a Macintosh or PC and selects from the periodic table the atoms for the molecule that is to be computed and visualized. A sequence of images can also be selected to allow for simple animations. Then the datafile created by Boogie is sent by modem or over the Internet to a remote supercomputer that is running NCSA DISCO, a chemistry solver that computes electron densities. Datafiles created by DISCO are then sent back to the user to be visualized with NCSA Collage or other visualization tools, such as Spyglass Transform or Dicer (which allows 3D animations).

With this approach, students and teachers using ChemViz materials become apprentice scientists rather than passive learners.

GalaxSee is an interactive tool for scientific inquiry that combines the power of a supercomputer with the user friendly environment of the Macintosh. It is designed to help young scientists investigate the

unresolved question: How do galaxies form? Although this question is typically studied only by research scientists, the combination of NCSA visualization applications written for the Macintosh with the accelerated calculations on the CRAY Y-MP supercomputing system invites even an elementary school student to ask the questions that contemporary scientists are asking.

With the GalaxSee program, the user specifies a number of stars, which the computer initializes in a random spherical distribution. The user then chooses the masses and velocities of these stars, and the computer takes it from there. At each time-step, the galaxy program simply calculates the force on each star due to all the others and then updates each velocity and position. The user can control how long the model runs and how often it updates the screen. The NCSA DataScope image window displays three perpendicular views of the galaxy—along the x, y, and z axes. Stars are represented as colored dots on the screen, with colors corresponding to the number of stars along the line of sight. Selecting an option in GalaxSee to generate an HDF (Hierarchical Data Format) file allows a stored movie to be made that can be animated with NCSA Image or NCSA Collage.

This program has been valuable for teaching modeling concepts to teachers and students. At first users simply change parameters allowed by the program, but they are encouraged to suggest new changes to the developers that can only be made by modifying the source code. They can then learn to modify code themselves to make the model behave as they want it to.

LaplaceSeein' combines a highly efficient implementation of a fast method on a supercomputer with the simple visualizations of the NCSA Scientific Visualization Software Suite to study electrostatic potentials and fields in the precollege curriculum. It is loosely based on the ideas Physics Professor David Renneke got from an NCSA workshop and uses in his classes at Augustana College [see *access*, April 1990].

The program can be used to study the potentials and fields near point charges, antennae, and arbitrarily shaped charged objects. Once the sys-

tem of charges and potential surfaces has been specified, users would like to know what the electrical potential looks like at every point in the sample volume. Of course, this could just be calculated directly at each point by integrating all charge contributions for all space at each point in space, but a much faster and widely used technique called the "relaxation method" is actually used to solve Laplace's equation.

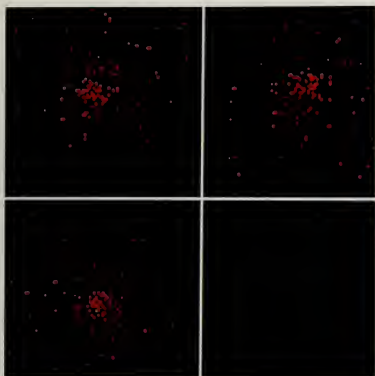
Laplace's equation describes the net curvature of the potential surface as zero everywhere in charge-free space. The relaxation method is very easy to understand, even for those who do not fully understand the equation it is solving. As an interactive process, each grid point is set equal to the average of its neighbors until convergence is reached. Laplace-Seein' displays the matrix of values representing the potential at regular intervals through the calculation in order to show the changes that are actually taking place and to show how the method converges to (or relaxes to) a solution. Using these visualizations, complex potentials can be easily constructed and compared.

The notebook feature of NCSA DataScope can be used to compute the electric field strength by evaluating the gradient of the potential. DataScope also allows for multiple visualization methods to be compared by the user.

SimSurface demonstrates two uses of scientific visualization. By animating a set of advanced numerical algorithms, a student can understand both the computational *process* and its result.

SimSurface demonstrates two common computational techniques: simulated annealing and the relaxation method. Simulated annealing is an often-used method for finding global maxima and minima of complicated or multidimensional functions. The problem being solved in SimSurface is a minimization of potential energy. The questions to be answered are: Given n stationary electrons confined to a 2D surface by four negatively charged walls, what arrangement of electrons has the minimum total energy? And is it the configuration preferred by nature?

The user can enter parameters that not only deal with the initial conditions of the surface and elec-



trons, but s/he can also adjust “knobs” for values that control the cooling process used by the simulated annealing algorithm. The program also displays the process of annealing at user-controlled intervals. This is an important aspect of the program. If it is to be used as a teaching tool—either for the physics or the numerical methods—it is instructive to watch as the minimization takes place. It is possible to see the electrons actually “freeze” into their lowest achievable energy configuration as the system cools. If the system cools slowly, the final energy is generally lower than a system that is quenched, or rapidly cooled.

Once the system has reached a minimum energy (to within a specified tolerance), the relaxation method is used to solve Laplace’s equation, and it is animated as it is in the LaplaceSeein’ solver.

SimElevator also uses simulated annealing, but it concentrates more on model building than model solution. The simulated annealing algorithm needs as its fundamental input a function that gets big when things go bad and gets small when the system is good. The goal is to help teachers and students understand how scientists come up with these “objective functions” that characterize a particular problem.

Elevators are common systems, so most students can easily relate to them. Simple observation leads us to conjecture that when individuals are in elevators they behave according to certain rules which can be modeled. For instance, some of us tend to avoid standing too close to the door or too



Simulations created using GalaxSee (left) and SimSurface (right) software developed by NCSA’s Education Group. (Courtesy of NCSA Education Group)

close to other people. This simulation allows users to set the level of “annoyance” created as more and more people enter an elevator. After seeing the results of the first trial, the levels can be modified or other factors can be added.

Fractal Microscope is an interactive tool designed by the NCSA Education Group for exploring the Mandelbrot set and other fractal patterns [see *access*, Fall 1993]. By combining supercomputing and networks with the simple interface of a Macintosh, students and teachers from all grade levels can engage in discovery-based exploration. This program can be used to introduce a wide variety of topics, including scientific notation, coordinate systems and graphing, complex numbers, and convergence and divergence.

Using these tools in the classroom

As part of its ongoing effort to train teachers, the Education Group offers a course called “Information Technologies for the Classroom.” Many teachers taking the course are incorporating the material into their lessons, developing lesson plans accessible from NCSA Mosaic, and making ambitious plans for the future.

In addition to the training provided by the Education Group, this course enables teachers to use the same tools, techniques, and technologies that scientists use. As their students begin to comprehend the “real” applications of the concepts learned in math and science classes, teachers can be assured that they have done their part to bridge the gap. By using supercomputers, the teachers have brought science as done by professional scientists to their classrooms.

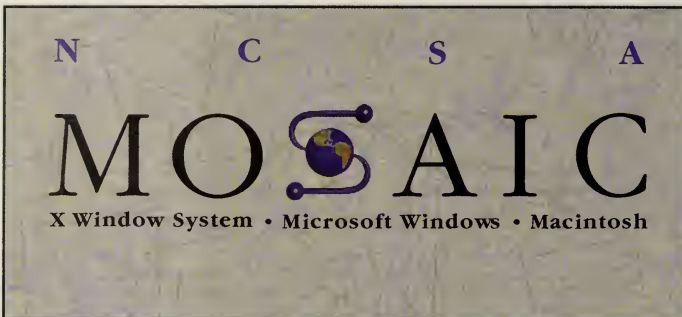
What is on the horizon for the BRIDGE Project? You guessed it—bridges! Among other ideas, several members of the group are already at work designing an interactive environment to enable students to delve into the science and engineering of building bridges. Cables, trusses, and the placement of supports will be part of the program.

Further information

If you are interested in obtaining more information about NCSA’s Education Program and its services, contact the Education Program (see *ncsa contacts*, page 2). ▲

USING NCSA MOSAIC

BY KENNETH CHANG, NCSA RESEARCH PROGRAMMER, PUBLICATIONS GROUP



NCSA Mosaic logo. (Design by Colleen Bushell, Research Programmer, SDG)

A wide variety of NCSA documentation, exhibits, and publications are available on your desktop via NCSA Mosaic, the latest software product of NCSA's Software Development Group [see *access*, Fall 1993]. Running on your local microcomputer or workstation, NCSA Mosaic can pull over information from NCSA's information servers on demand.

What's available

Here's a partial listing of information available through NCSA Mosaic:

- **Documentation**—User guides for NCSA's CONVEX C3, CRAY Y-MP, and Connection Machine (CM-2 and CM-5) computers. Also available are user guides for the UniTree mass storage facility and AFS (Andrew File System).
- **General information**—How to apply for time on NCSA's computers; NCSA policies and services.
- **Technical reports, preprints, and reprints**—Research reports by NCSA staff.

- **Technical Resources Catalog**—Listing of manuals, software, and other products available from NCSA.
- **access**—Online, hypermedia version of the publication you are reading.
- **Calendar of MetaCenter events**—List of workshops, deadlines, conferences, classes at the five NSF MetaCenter supercomputing sites.
- **Overview of NCSA**—Information about NCSA groups, projects, and affiliated organizations.
- **Hypermedia exhibits**—Online exhibits including a tutorial on fractals, an Internet version of the NCSA Digital Gallery CD-ROM, an introduction to the UIUC, and an art exhibit from the university's Krannert Art Museum.

How to get NCSA Mosaic

NCSA Mosaic is available via anonymous FTP from <ftp.ncsa.uiuc.edu>. See the inside back cover of this publication for detailed instructions. There are three flavors of NCSA Mosaic: NCSA Mosaic for the X Window

System (or X), NCSA Mosaic for Macintosh, and NCSA Mosaic for Microsoft Windows.

Getting to NCSA's Home Page

Once you have successfully installed NCSA Mosaic, your initial "home page" (that is, the document that is displayed when you start up the program) is the NCSA Mosaic Home Page. This page provides general information about the software and some general jumping off points for exploring the Internet.

To get to the NCSA Home Page, the simplest means is to click on "NCSA." Alternatively, you can select **Open URL . . .** from the **File** menu and then enter <http://www.ncsa.uiuc.edu/General/NCSAHome.html>

From the NCSA Home Page, all of the information described above is available through a few mouse clicks.

Setting the NCSA Home Page as your home page

You can set your default home page to be the NCSA Home Page. This can be convenient if you access NCSA information often.

- **X Window System version**—In your `.cshrc` file, add the line `setenv WWW_HOME "http://www.ncsa.uiuc.edu/General/NCSAHome.html"`
- **Macintosh version**—Select **Preferences** from the **Options** menu, then in the **Home Page** field, type <http://www.ncsa.uiuc.edu/General/NCSAHome.html>
- **Microsoft Windows version**—In the `MOSAIC.INI` file, there's a line that starts with "Home Page =". Edit this line to read:
Home Page="http://www.ncsa.uiuc.edu/General/NCSAHome.html" ▲

NCSA MOSAIC UPDATE

Worldwide interest in NCSA Mosaic continues to grow. We are sorry if you have been experiencing slow connect time. The server has been extremely busy due to user interest. During one week in February alone, there were 1,153,843 connections. From September through November 1993, over 34,000 copies of the X Window System version were downloaded from the NCSA server. This amount is more than had been downloaded during the previous six months. Over 31,000 copies of the Macintosh version and over 13,000 copies of the Microsoft Windows version were downloaded during the same time. Roughly half of this activity was from mid-October to mid-November.

NCSA Mosaic downloads by month

	X	Mac	PC
January 93	145	-	-
February	1,661	-	-
March	4,473	-	-
April	5,014	-	-
May	3,110	-	-
June	5,098	-	-
July	5,511	-	-
August	4,634	-	-
September	6,632	4,834	732
October	11,236	10,790	4,348
November	16,649	15,477	8,421
December	19,630	13,827	7,706
January 94	16,310	13,927	9,050
February	<u>21,390</u>	<u>13,508</u>	<u>17,202</u>
Totals	121,493	72,363	47,459

All three platforms had a major release during the first two weeks of November 1993 with the X Window System client going to Version 2.0, and the Mac and Windows clients going to Version 1.0 full releases. The Mac and Windows clients were not released until September 1993.

▲

NCSA MOSAIC CONFERENCE

The worldwide use of NCSA Mosaic and other NCSA software has sparked interest in a software user conference. In response to that interest, NCSA's Software Development Group is planning an information technologies conference with a focus on NCSA Mosaic—possibly including presentations on Collage and HDF. It is scheduled to be held in Chicago mid-October, 1994. We will let you know the details as plans develop.

You may help determine the topics for the conference. Take a look at the topics listed online and tell us which ones would be of interest to you. List other topics that you think would be of use to a number of people.

You can see the list of possible topics on the World Wide Web server. Refer to the inside back cover of this publication for the IP address. The list is also available via anonymous FTP by entering `/ncsapubs/IT94/IT94.txt`.

Send your queries, responses, and suggestions to `citconf94@ncsa.uiuc.edu` (Internet).

NEW FORUM FOR FINITE ELEMENT USERS BY MINAZ PUNJANI, UNIVERSITY OF LONDON COMPUTER CENTRE

FEUSERS is a mailbase-list serving researchers, teachers, and groups active in using and developing finite element and finite difference software. Code developers and vendors of these packages are particularly encouraged to be involved in FEUSERS.

Users and developers of graphical pre- and postprocessing systems (with solid modeling) and CAD/CAM interfaces for finite element and finite difference applications software are also encouraged to participate. Industrial participants with a solutions approach would also be appreciated.

The FEUSERS forum aims to encourage discussion and free exchange of ideas amongst members. All postings to the group are distributed to all the list members. Initially, the list will not be moderated.

To join the list and become a list member of FEUSERS, email the following single line:

JOIN feusers YOUR_Firstname Your_Surname to
mailbase@mailbase.ac.uk

To contribute to the forum, email the item to:
feusers@mailbase.ac.uk

—from Minaz Punjani, Engineering Computing, University of London Computer Centre, 20 Guilford Street, London WC1N 1DZ, United Kingdom; Phone: [+44] 071 405 8400; FAX: [+44] 71 242 1845; email: m.punjani@ulcc.ac.uk (Internet) or m.punjani@uk.ac.ulcc (Janet). ▲

FLASH! NCSA MOSAIC LICENSES SIGNED BY JARRETT COHEN, STAFF ASSOCIATE, DIRECTOR'S OFFICE

As of late March, five companies have signed the first licenses to distribute NCSA Mosaic and incorporate it into their products. They are Quarterdeck Office Systems Inc., Santa Monica, CA; The Santa Cruz Operation, Inc., Santa Cruz, CA; InfoSeek Corp., Santa Clara, CA; SPRY, Inc., Seattle, WA; and Quadralay Corp., Austin, TX.

NCSA Mosaic is free for academic, research, and internal business purposes. Nonexclusive licenses are necessary for commercial use and redistribution. Licenses can be written for one version or all three versions of NCSA Mosaic. Companies have the option of using updates as they become available.

The center is negotiating with a few dozen other companies. NCSA has had over 100 commercial contacts for licensing the software, said Joseph Hardin, associate director, Software Development Group. ▲

PVM PROJECTS ON NCSA'S HP CLUSTER

In the last issue of *access* [see *access*, Fall 1993], NCSA's new high-performance Hewlett-Packard (HP) cluster of workstations was announced.

Configuration

The current HP cluster consists of a model 715 file server and eight model 735 compute nodes. The cluster is configured with the 715 as the interactive machine that provides an environment for tasks such as software development, compiling, debugging, and file management. The eight 735s are used as compute servers.

The Parallel Virtual Machine (PVM) distributed processing package has been chosen as the software on the HP cluster for porting parallel applications. PVM is becoming the de facto standard among message-passing libraries due to its widespread usage and its support by many major computer vendors.

Access to the compute servers is only available through the DQS batch system, consisting of two queues on each of the compute servers—one serial and one parallel. The serial queues are subordinate to the parallel queues, allowing jobs requesting parallel queues to have priority. The compute servers share the same root file system as the 715. The Network File System (NFS) is used to share user home directories and other file systems.

Reports from users

NCSA Research Programmer John Quinn is overseeing work on the HP cluster and is advising users on PVM. Quinn recently solicited some comments from early users.



Atmospheric sciences—NCSA Research Programmer in Applications **Crystal Shaw** says: "We are planning to make high-resolution 2D and 3D nested-grid simulations of intensifying cold fronts and associated thunderstorm development. We hope to (1) benchmark the COMMAS model on a single-processor HP machine, and (2) investigate the feasibility of using the entire cluster, and compare the performance to COMMAS run on a single CRAY Y-MP processor and to COMMAS on the 8-processor CONVEX C3880."

Engineering sciences—NCSA Research Scientist **Danesh Tafti**, (Applications) and **Weicheng Huang** (NCSA graduate research assistant) report: "Work is being performed to evaluate the message-passing paradigm via PVM for the time-dependent solution of the incompressible Navier-Stokes equations for direct numerical simulations of turbulence. Our current focus is on the NCSA HP-cluster, but the codes developed using this protocol will be portable to other distributed memory systems which run PVM."



NCSA's HP cluster (Photo by Wilmer Zehr)



Engineering—NCSA Programmer **Mark Straka** (Applications), who is working with NCSA industrial partner Caterpillar says: "I am exploring the use of the PVM library on the HP cluster as a means of distributing the memory and computational workload for a 3D analysis code. Caterpillar Inc., to which this code is proprietary, hopes to soon bring the software developed at NCSA back to its local computing facilities. With the recent and rapid advances in the speed of workstations, it is now possible for a research engineer to have the power of a 100 Mflop 'supercomputer' in the office. A distributed cluster of such workstations may very well be the most cost-effective environment for solving problems with a significant amount of task or data parallelism.

"Since PVM is portable and easily installable, Caterpillar may ultimately be able to harness the power of several workstations configured with PVM and bring them to bear on larger simulations, solving larger problems in a fraction of the previous time. This is an attractive pursuit for Caterpillar since it has the potential for providing them with both 'supercomputer' power and local flexibility under their own control. PVM provides users with the flexibility to dynamically configure the available CPUs on a network so that the start-to-finish run time can be minimized—in contrast to the often frustrating experience of waiting in queues with poor turnaround time on the monolithic traditional supercomputers.

"Work is still being done to analyze the performance of the FDDI interconnect between the eight HP 735s in the cluster, and whether the bandwidth of the PVM communication library and underlying hardware will support the amount of data that needs to be moved in this particular application code. More timings and comparisons (against the nondistributed code) need to be completed before any speedup ratio can be quoted. The overhead factor involved with distributing the data for this particular code will be the key in deciding the viability of this approach,

particularly in determining what number of processors is optimal."

V. Varadarajan, UIUC Department of Electrical and Computer Engineering, says: "We have developed PVM codes for conjugate gradient method algorithms. We find that good parallelism exists for large problems that are of interest to us. We have also developed finite-difference time-domain codes using PVM. We find that at 14 Mflops per process, eight processors can give linear speedup for certain problem sizes. Now we have fine-tuned codes that can run at 35 Mflops per processor. This means that we can get the performance of a CRAY C90 processor for our algorithm. Note that the CRAY C90 gives only about 300 Mflops for our problem. Eight HP-735s can give 280 Mflops for our problem in single precision.

"At high Mflops our codes require [a] high-speed network. Ethernet is not good enough, since we have to exchange more than 4x104 words between every two processors in each iteration. . . . We find that large problems can be finished within 10 to 15 hours using eight HP 735s."



Materials science—William Magro (NCSA Research Assistant, Applications) who collaborates with his advisor **David Ceperley** (Quantum Systems team leader and research scientist) says: "I have used the HP cluster, along with my 386 PC running Linux (a free UNIX), to develop and debug a parallel PVM-based version of our group's Path Integral Monte Carlo (PIMC) program.

"PIMC is a statistical approach to thermodynamic problems in quantum many-body physics. PIMC can be parallelized on two levels. First, on an algorithmic level, multiple nodes can collaborate on a simulation. Second, because of the statistical nature of Monte Carlo techniques, we can achieve perfect scalability in a parallel environment by running several statistically independent simulations in parallel. The two approaches can be used at the same time. The algorithmic approach is more complicated and is the focus of the current work. The statistical approach has been implemented. The code is currently being used to

calculate properties of a hydrogen plasma near the $H_2 \rightarrow 2p^+ + 2e^-$ phase transition.

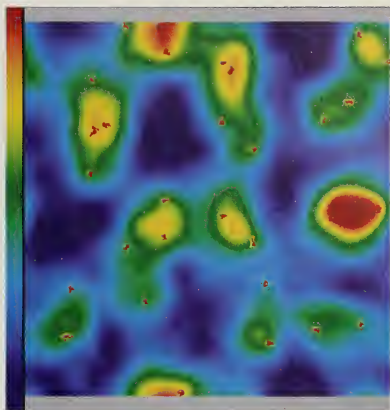
"I have written a visualization program to complement the PIMC code." See Magro's visualization of molecular hydrogen (right).



Other users—NCSA Research Scientist and Mathematics and Computer Science team leader Michael Heath has used the HPs to port and verify the performance of his latest release of ParaGraph software application [see *access*, January–April 1992]. The software provides detailed, dynamic graphical animation of the behavior of parallel algorithms, as well as graphical summaries of their performance.

Angie Mounts of United Technologies Research Center (UTRC) spent three weeks at NCSA working on HP cluster infrastructure issues, parallelizing and benchmarking some of UTRC's codes. Mounts is a researcher with NCSA's newest industrial partner, United Technologies Corp.

Kevin Chang (FMC), another NCSA industrial partner, parallelized and benchmarked some of FMC's codes on the cluster. ▲



Snapshot of a molecular hydrogen simulation at 6,250 K. In this 2D projection of a cube, purple indicates low density and red, high density. Compact red objects are protons; green to red areas represent electron clouds binding the protons. (Courtesy William Magro)

HELICAL SCAN TAPE DRIVE AVAILABLE BY **ROBERT E. MCGRATH**, RESEARCH PROGRAMMER, COMPUTING AND COMMUNICATIONS GROUP

NCSA has one high-speed, high-capacity Ampex DD-2 helical scan tape drive installed as a normal tape peripheral on NCSA's CONVEX C3880. It is now available for use. The DD-2 is not integrated into the existing Mass Storage System hierarchy, so access to it is not transparent.

A document called "Using the DD-2 Drive at NCSA" explains the current configuration of the DD-2 drive and how to use it. It is available in postscript (laser printer ready) on the CM-5 in /usr/doc/Dd2UserNotes.ps, on the C3 in /ncsainfo/Dd2UserNotes.ps., or via the Internet (see email address below).

What is the DD-2 drive? The DD-2 drive is a modified videotape recording system that provides high-capacity, relatively high-speed storage. NCSA's "small" DD-2 tape cartridge holds 25 gigabytes. The transfer rate varies, but it should be at least 4 megabytes per second. The DD-2 drive is only accessible from the CONVEX C3880, so data must be transferred from other systems to local disk on the Convex system before storing it on DD-2 tape.

Who may use the DD-2 drive? Users with very large datasets (1 gigabyte or more) should consider using DD-2 tape, particularly if the data can be written in 1 megabyte chunks. The DD-2 drive is not very useful for storing large numbers of small files.

How can I use the DD-2 tapes? (1) Get the document "Using the DD-2 Drive at NCSA" as described above. (2) Contact NCSA help desk (see email address below) to obtain tapes and login information. (3) Reserve disk space and the DD-2 drive for exclusive access when needed. (4) Transfer data to the Convex system, and then write it to tape with tar.

To obtain more information, contact help@ncsa.uiuc.edu or mcgrath@ncsa.uiuc.edu (Internet).

the advanced teleconferencing facilities are in place, the group will have what Schulten calls a "teleacademy" for computational biology.

Enhanced communication in the field, as well as the development and dissemination of new algorithms, lays the groundwork for breakthrough achievements in molecular biology. "The core Grand Challenge goal," says Schulten, "is to do research with these high-performance computers that could not be done otherwise."

New research on proteins

New research will describe proteins interacting with membranes and with DNA, and the complete poliovirus coat. "You can think of the virus as being the most primitive animal. It is in some ways a complete living entity. . . . What you have here is, for the first time, an attempt to describe a complete living system on the atomic level."

Collaborators on the NSF-funded project, in addition to Brünger, include John Arnold Board, Jr., Duke University; Laxmikant Kale and Robert Skeel, UIUC; and Tamar Schlick, New York University. ▲

Universe continued from page 16

grids at various levels of the hierarchy. What has happened is that this system has spawned all of these calculations, but these calculations are not independent. The boxes need to know what is going on in their neighbors' [boxes].

"The grids adapt hierarchically to resolve new structures, but they also adapt in the sense of tracking features," Norman says. "For instance, if a galaxy were moving, a subgrid would move with it."

A computer science challenge

"Programming [this problem] involves creation and management of a complex hierarchical adaptive data structure. That is how a computer scientist looks at this," Norman says.

HAMR must manage the grid hierarchy, but "What equations are actually being solved on these grids?" Norman asks. "So far, they are just the lattices. To make HAMR application-specific, it is necessary to tell it what equations to solve on each grid. Furthermore, you have to tell it the boundary conditions of each grid.

"To construct a hierarchical adaptive mesh application, you need two neatly divided pieces: an adaptive mesh refinement system that is application-independent and physics solvers," Norman states. Neeman is developing the first, HAMR. Bryan is developing physics solvers that will constitute NC Hammer.

Using HAMR's approach results in huge memory savings, Norman says. "It takes the completely impossible and makes it possible. The price to pay is that hierarchical adaptive mesh refinement is complicated.

"The computer science challenge along with the [science] Grand Challenge is how to implement HAMR on the CM-5," Norman says, stressing

that researchers need a completely new programming language. As of early 1994, Norman says his group has the physics solvers (CMHOG, KRONOS) running on the CM-5 and that HAMR is almost running on conventional supercomputers.

"The Grand Challenge of cosmology is one of the thrusts that marry the two," Norman says. ▲

NCSA REFUND POLICY AND PROCEDURE

BY JOHN TOWNS, NCSA TEAM LEADER, CONSULTING

Policy for granting or denying a refund request

A refund request will be considered when one of the following is true:

1. Output was lost because of a system crash.
2. A bug in system software caused incorrect output.
3. NCSA staff gave misleading advice, causing incorrect output.

Refund requests will be denied when one of the following is true:

1. Less than X_{machine} Service Units (SU) were consumed (academic users only), where:
 - X_{CM-5} = 2.0
 - X_{YMP} = 0.5
 - X_{C3} = 0.5
2. The request was made more than two weeks after the charge.
3. No charges were recorded for the job in question. (If the system crashes before a job finishes, the CPU usage will not be recorded in the accounting file.)

Procedure for handling refund requests

The user makes the request to the consulting staff. (Academic users contact the National Consulting Office; industrial users contact their assigned consultant.)

The user should provide as much information as possible. The list below shows the minimum information required. Additional information may include error messages displayed or a copy of the batch script used.

- User ID
- Machine
- Date that the job finished
- Reason for the request
- DJM/NQS request ID

NEW SOFTWARE ON CONVEX

C3880 BY DAVID McWILLIAMS,
NCSA RESEARCH PROGRAMMER,
COMPUTING AND COMMUNICATIONS

The following new software has been installed on the CONVEX C3880:

CONVEX CXwindows Version 3.1
CONVEX CXwindows 3.1 upgrades OSF Motif from version 1.1 to Version 1.2 and fixes bugs in the X programming libraries and clients. CONVEX CXwindows 3.1 also adds PEXlib, the X Consortium sample implementation programming library that generates PEX 5.1 protocol. All software in the CONVEX CXwindows 3.1 release is based on X Version 11 Release 5, OSF/Motif Version 1.2, and ANSI C.

NOTE: For more information, see the file /usr/doc/CXwindows.3.1.relnotes.

Convex Performance Analyzer (CXpa) Version 2.0

CXpa is a performance analyzer for C, Fortran, and Ada that allows users to profile optimized programs compiled with one of the profiling flags (-pa, -par, -pab). CXpa can run under CXwindows or with terminals such as a vt100.

NOTE: For more information, see /usr/doc/v2.0cxpa.relnotes.

Convex AVS Applications Version 1.0

Convex AVS Applications 1.0 is a release consisting of new and enhanced modules in finite element analysis, protein chemistry, and quantum chemistry.

NOTE: For more information, see /usr/doc/V1.0ConvexAVS_Applications.relnotes.

Convex AVS Version 5.0

Convex AVS V5.0 includes many new features, including hierarchical networks or "macro modules," enhanced flow executive, and a software renderer. The Data Viewer Application provides a simpler interface to those users who are mainly interested in quickly looking at their data and not in developing networks of AVS modules.

NOTE: For more information, see /usr/doc/V5.0ConvexAVS. ▲



NCSA recently enjoyed a visit from Xavier Rodet (right) from IRCAM (Institute for Research and Coordination of Acoustics and Music), Paris, France. Rodet is one of the leading audioengineering researchers in signal processing and physically based models for sound synthesis and musical applications. Robin Bargar (left), member of the Virtual Environment Group, gave Rodet a tour of NCSA's facilities. The two met to discuss continuation of software and sound synthesis collaborations that they initiated at CNMAT (Center for New Music and Audio Technologies), University of California, Berkeley. (Photo by Thompson-McClellan Photography)

Quantum continued from page 7

Three QMC codes have been ported to the CM-5 for use in the MIMD mode. Each node does a separate Monte Carlo simulation for a time, then the results are averaged to achieve higher accuracy. This strategy results in much lower internode communication.

When the full 512 nodes are used, the Path Integral Monte Carlo code gets a floating point speed of 15 Gflops.

Gaining speed through advancements in technology is of great interest to Ceperley's group. "Obviously, we are planning to have much more powerful computers available in the next few years," he says. "This will enable us to 'solve' many of the long-standing problems in condensed matter physics, or more modestly, to provide a new way of understanding them or calculating properties." ▲

Radio synthesis continued from page 10

Utilizing the CM-5

As with deconvolution, self-calibration calculations are ideally suited to the CM-5's scalable system at NCSA. "The reason we can use parallel processing effectively is due to the fact that different parts of the computation are largely independent," says Crutcher. "That's easy to partition among the various processors."

By obtaining access to NCSA's metacomputer, Crutcher can now create an image with better resolution in much less time. Astronomers will soon be able to spend their time trying to understand what their data reveals of the universe, rather than waiting for insufficient computer resources to process the data. ▲

EXPLORING CYBERSPACE

BY KENNETH CHANG, NCSA RESEARCH PROGRAMMER, PUBLICATIONS GROUP

... And in the bloodlit dark behind his eyes, silver phosphenes boiling in from the edge of space, hypnagogic images jerking past like film compiled from random frames. Symbols, figures, faces, a blurred, fragmented mandala of visual information.

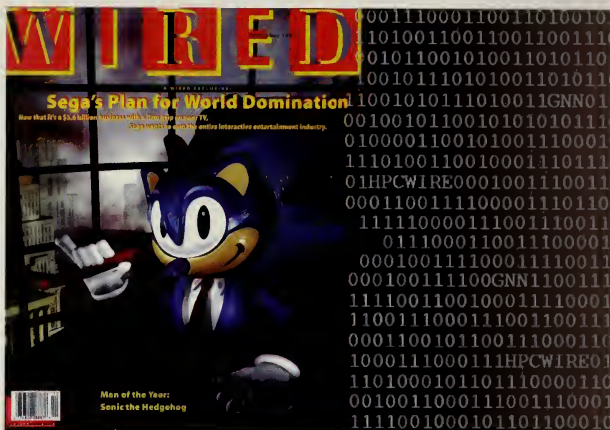
—from *Neuromancer*
by William Gibson

Nearly a decade ago, when people were busy comparing how 1984 had not turned out like 1984, out came William Gibson's *Neuromancer*, a vision of a high-tech dystopia where virtual reality was more compelling and immediate than the decaying physical world. The novel launched a term and fiction genre—cyberspace and cyberpunk, respectively—as writers speculated on life “jacked” into a computer network.

Today, with the Internet connecting millions across the world, reality is taking the first steps towards cyberspace. The interface is still through pictures and words on a cathode ray tube rather than optical fiber from neuron to silicon, but already there is a distinct online community and culture.

Enter *Wired* magazine. Succinctly: if cyberspace were a magazine, it would be *Wired*.

“Our mission,” writes editor/publisher Louis Rossetto in the November 1993 issue, “is to cover the biggest story of the decade—the convergence of computing, telecommunications, and the media—for the most powerful people on the planet today, the people making this Digital Revolution.”



Nine issues into its existence, *Wired* succeeds. First, it is visually vibrant. Innovative, brash, and using nearly as many neon colors as you'd find on Venice Beach, the graphic design is almost a pictorial representation of cyberspace. It works most of the time, too. (Occasionally, it goes too far. An interview with Alvin Toffler, for instance, is printed as black and red text on a bright yellow page. That's guaranteed to give you a headache even before you get to the part where Toffler predicts personal nuclear weapons.)

Second, the articles are very good, covering the range of issues involving the new electronic media and not just the technology. In a recent issue, Mitchell Kapur, who founded Lotus, discusses the politics of access to the up-and-coming “information superhighway.” There's an article about the patchwork of computer networks sprouting in Russia now; another about Iridium, Motorola's satellite-based phone system.

Image by Linda Jackson; concept by Kenneth Chang (December 1993 cover adapted with permission from *Wired*)

The magazine mixes the familiar with the unexpected. There's a piece by William Gibson in the September-October 1993 issue. But instead of something predictable like another article about cyberpunk, he reports on Sing-a-pore, a squeaky clean country ruled by benevolent paternalism. (“If IBM had ever bothered to actually possess a physical country,” Gibson states “that country might have had a lot in common with Singapore.”)

Wired's shorter pieces survey the panorama of technological eclectica (a virtual skiing lab in Tokyo, next-generation ovens that use high-powered lights to cook a steak in slightly more than a minute and a half), the latest jargon (“**net spider**—someone who spends a lot of time scrambling from

one computer net to another”), and little gems on the Internet such as: *Stressed-out by the pace of Net.Life? Why not telnet to cheshire.oxv.edu 7777—when you do, this calming incantation will appear: “Amid the smell of incense and the sound of gongs and chanting, you have come upon the glorious Zen MOO. Please be quiet and enjoy your meditation.”*

Two other publications explore some of the potential of electronic media. *HPCwire: The Electronic News Magazine for High-Performance Computing* is described by its name. Compared to *Wired*, *HPCwire* is plain. The format is simple ASCII text wrapped at 80 columns so it can be read on any computer terminal. The articles aren't breezy prose, either. Many appear to be rewritten press releases.

But flashy layout and breezy prose aren't the purpose of *HPCwire*. Rather, it's a one-stop way of staying informed with the developments in high-performance computing. Each week, the 11,000+ subscribers receive in their electronic mailboxes the table of contents of the latest issue, a series of one-or-two line summaries of that week's news and feature articles. If an abstract catches one's fancy, the complete article can be quickly ordered via email. The table of contents of a recent issue included “SDSC Doubles Speed and Memory of New Cray Research C90,” and “Maspar to Reorganize as Part of New Target Market Strategy.”

There are some general articles often reprinted from the *Wall Street Journal*, *Science*, and other publications, but *HPCwire* is first and foremost a compendium of high-performance computing news. If your job or interests overlap with its contents, *HPCwire* can be a valuable resource.

Something closer to the future is *GNN Magazine*, published by O'Reilly and Associates. (GNN is short for Global Network Navigator.) To read it, you first need a connection to the Internet and second, NCSA Mosaic.

Once you have those two things, you can start reading. NCSA Mosaic allows both formatted text and images, so reading the computer screen is roughly the same as reading a printed magazine. In content and in purpose, *GNN Magazine* appears similar to *Wired*. In its premiere

issue of October 1993, there is an article about Mitchell Kapor (reprinted from *The New Republic*) that covers much of the same ground as Kapor's piece in *Wired*. Another piece provides a good overview of the Internet (reprinted from *The Nation*). Among other things, there is a humorous article about the White House's foray into email and form letters, short opinion pieces from people setting up community networks across the country, and an art gallery.

The writing is a bit dry in places, and the overall feel is more of a magazine that has been ported online than an online magazine. That's a bit harsher than I mean. *GNN Magazine* is already one of the nicest displays you can find with NCSA Mosaic, but it's also clear that people are just learning the new media's strengths and how to take advantage of them.

GNN Magazine is well worth the visit. (For those who have NCSA Mosaic, the URL is <http://nearnet.gnn.com/mag/demo.toc.html>) *GNN Magazine* is free, though O'Reilly asks that you become a registered reader. Send email to info@gnn.com for details.

The subscription rate for *Wired* is \$39.95 for 1 year (12 issues). Call 1-800-SOWIRED or email subscriptions@wired.com for more information. *Wired* is available online on the World Wide Web. (The URL is <http://www.ncb.gov.sg/WoWWW.html>)

HPCwire's annual rate is \$195. If you are a student or if you will be an added subscriber at your site, your annual rate is \$59. Send email to sub@hpcwire.ans.net for more information. ▲

NCSA MOSAIC WINS IMA AWARD

Internet Multicasting Service recently announced 1993 Ima Award winners.

The awards are given to “recognize people, software, and computers that have made a significant contribution to the Internet.”

NCSA Mosaic won the award for “Most Innovative Application.” The award citation follows:

“This ‘Ima’ Award is presented to NCSA Mosaic in the category of ‘Most Innovative Application.’ 1993 has been the year of the Internet Application, but the National Center for Supercomputer Applications has risen above this distinguished fray to develop a truly impressive piece of programming. NCSA Mosaic, which runs on X Windows, the Macintosh, and Microsoft Windows, is an interface to the World Wide Web, but has also integrated transparent access to other Internet services, ranging from FTP to WAIS to Gopher. NCSA Mosaic, in addition to an unparalleled flexibility in design, has proven to be a superb implementation.”

Other winners and their categories included Tim Berners-Lee and the World Wide Web Team, most innovative architecture; and O'Reilly & Associates Inc., most exhaustive documentation (see book review). One of three honorable mention awards went to *Wired* “for the coolest new magazine.” *Wired* is reviewed beginning on the opposite page.

Ima Award winners are selected annually by Internet Multicasting Service's Prize Committee, an anonymous group of Internet users and developers. Award categories will vary each year.

MILESTONES

Staff Changes

Lex Lane is associate director for User Services and Educational Outreach (USEO). Lane has a strong background in user support and has performed a variety of roles at the center.

Radha Nandkumar, who has served in the Director's Office for several years, has joined USEO in a move that consolidates user allocation services. Her functions with user project proposals, Peer Review Board processes, and grant allocations will be joined with those of the Client Administration Group.

John Towns, researcher with the Gravitation Group, is team leader of Consulting. Since joining NCSA in 1989, Towns has collaborated with various groups at the center. His emphasis has been on improving the Consulting Program's relationship with the national user community.

Sabbatical leave

Donna Cox is taking a one-year sabbatical from her position at NCSA to work with **Thomas DeFanti**, visiting associate director for the Virtual Environments Group (VEG) [see *access*, Fall 1993]. They will be merging high-end visualization research and production with virtual environments.

During his one-year appointment at NCSA, DeFanti will remain professor of electrical engineering and computer science and co-director

of the Electronic Visualization Laboratory (EVL) at UIC.

Moving on

David Bernstein, former postdoctoral research associate in the Gravitation Group, moved to Australia. As a postdoctoral associate at the University of New England, Armidale, New South Wales, he continues working in numerical relativity and black holes. Bernstein came to NCSA in its earliest days as a graduate student collaborating with NCSA Director Larry Smarr.

In April 1994 **Jarrett Cohen** left NCSA to become senior publications specialist at Hughes STX Corp., a contractor to NASA Goddard Space Flight Center, Greenbelt, MD. Cohen, who was at NCSA 6 years, started as a student in the Publications Group and later became NCSA's Public Information Officer. He wrote for *access*.

Barbara Mihalas, former research scientist in the Applications Group, is a senior research scientist and associate director at Syracuse University's Northeast Parallel Architectures Center. Her new duties include education and industrial outreach.

Robert Patterson and **Michael McNeill**, former NCSA visualization specialists, recently joined Industrial Light and Magic in California.

New appointments

Orville Vernon Burton, NCSA principal investigator and UIUC history professor, has been appointed to the Center for Advanced



Barbara Mihalas, left, and Crystal Shaw (NCSA research programmer) at the farewell party for Mihalas. (Photo by Vincent Jurgens, VEG)

Study for the 1994-95 academic year. The grant allows more time for scholarly research.

Michael Heath, leader of NCSA's Mathematics and Computer Science team in the Applications Group, was appointed to the UIUC Steering Committee for the Computational Science and Engineering Program by Dean William Schowalter, College of Engineering. Heath is subject area editor of linear algebra and visualization for the *International Journal of Supercomputer Applications*.

Bruce Schatz became a research scientist at NCSA and a UIUC associate professor in the Graduate School of Library and Information Science at the beginning of the 1993-94 academic year. Schatz is nationally recognized for his development of new technology for digital libraries and their elec-

tronic deployment to the scientific community.

Awards

InfoWorld's editors named **NCSA Mosaic** 1993 Product of the Year in the Bob Metcalfe's Industry Achievement Award category. Each year the publication awards achievement in 11 categories of personal computer hardware, software, and networking products. See the next issue of *access* for more information.

Doug Swesty, UIUC postdoctoral research associate in Applications, received an NSF Advanced Scientific Computing Fellowship to model the explosion mechanism of type II supernovae using numerical radiation-hydrodynamic simulations with scalable HPCC codes.

A Global Solution [see *access*, Spring 1993], the MetaCenter videotape for outreach to U.S. business, was a finalist in the 1993

New York Festivals Awards Competition for Television Programming and Promotion Nonbroadcast Film and Video. **David Curtis**, creative director, wrote, directed, and produced the video. Others cited include: **Robert Patterson**, designer and online editor; **Tony Baylis**, videographer; **Robin Bargar**, composer; and **Jay Rosenstein**, audio technician.

access won a second place award of merit for editorial content in the 1993 Central Illinois Master Communicator competition. **Fran Bond**, editor; **Melissa Johnson**, managing editor; and **Linda Jackson**, designer, were recognized in the magazine publication category by the sponsoring societies: the International Association of Business Communicators, the Public Relations Society of America, and Women in Communications.

Milestones continued on page 36

SMARR BECOMES FELLOW

NCSA Director Larry Smarr was elected a Fellow of the American Academy of Arts and Sciences March 9, 1994. New members are elected by the current membership in recognition of distinguished contributions in their fields. Smarr was chosen for his efforts in Educational and Scientific Administration.

Founded in 1780, the academy honors achievement in science, scholarship, the arts, and public affairs. It conducts a varied program of studies that reflects the interests of its members and is responsive to the needs and problems of society and of the intellectual community.



U.S. Congressman Tom Ewing (15th District) visited NCSA recently and saw demonstrations of NCSA Mosaic and Caterpillar's virtual reality project. Ewing "rode" Caterpillar's wheel loader in the Virtual Reality Laboratory as members of the project team looked on: (left) Dee Chapman, NCSA industrial consultant to Caterpillar, and (right) Matthew Vande Wiele, NCSA consulting engineer. (Photo by Tony Baylis, USEO)

NSF EFFORTS RECEIVE HIGH PROFILE AT SUPERCOMPUTING '93

BY JARRETT COHEN, STAFF ASSOCIATE, DIRECTOR'S OFFICE

Over 5,200 people attended Supercomputing '93, November 15-19 in Portland, OR. Conference chair was Robert Borchers, director of NSF's Division of Advanced Scientific Computing.

Keynote address

Recent appointee at NSF, Director Neal Lane, delivered the keynote address. Among his topics were a perspective on NSF's role in HPCC and a vision for the future.

"Looking back after a decade, we can now ask ourselves if the program fulfilled its promise and met its goals," Lane said. "The results speak for

themselves—or I should say, yourselves."

He pointed out the accomplishments of the NSF supercomputer centers, including the support of over 15,000 researchers, the development of many powerful tools, the growth of NSFNET, and the building of 80 industry partnerships.

For the future, Lane gave attendees two starting points for reaching the next level of success, the Branscomb Report and the *National Information Infrastructure: Agenda for Action*.

The Branscomb Report is the popular name for a report given by an NSF-convened blue ribbon panel, chaired by Lewis Branscomb

of Harvard. *From Desktop to Teraflop: Exploiting the U.S. Lead in High Performance Computing* is its full title.

"The report calls upon NSF to achieve a better balance in its distribution of resources," Lane said. "It uses the image of a pyramid to describe the ideal balance. At the base of the pyramid would be powerful workstations for individual users. The second tier would include midrange machines that would serve academic departments and large laboratories. The third tier would contain supercomputers. And at the apex of the pyramid would be the highest level of computing power available, presumably a teraflop facility."

Lane sees the NII *Agenda for Action* as an even broader vision statement. The NII "is intended to provide all Americans with the ability to access a wealth of information and to communicate with one another using voice, video, images, and data."

MetaCenter exhibit

Research exhibits afford supercomputer centers, laboratories, and universities the opportunity to present demonstrations and information. The National MetaCenter, along with NCAR, collaborated on its third exhibit.

The centers highlighted their collaborations through a diversity of workstation-based demonstrations and videotapes.

NCSA showcased two projects. *The Relativity Workbench* is a distributed tool for computing solutions to the Einstein equations through an intuitive visual user interface. It was developed by Daniel Weber, NCSA research programmer; George Heinz, former

Supercomputing '93 continued on page 36

REL VISITORS FROM ABROAD

BY PAULETTE SANCKEN, NCSA PUBLIC INFORMATION
SPECIALIST, PUBLICATIONS GROUP



Donna Cox (member of NCSA's Virtual Environments Group and UIUC Art and Design professor) has hosted a number of guests in recent months via the Fine and Applied Arts Visitors Program.

Coming to NCSA through an informal applications process, artists are guaranteed access to some of the highest quality facilities for computational image-making in the world at NCSA's Renaissance Experimental Laboratory (REL).

"The convergence of art and science is virtually a reality at NCSA, a place where disciplines and individuals can interact in one of the highest-tech environments in the world," Cox says.

Visitors during the fall semester of 1993 follow.

Robyn Stacey is visiting NCSA from the University of West Sydney, Australia, where she teaches photomedia in the design department. "I am interested in the way science impacts on and shapes our lives and pre-determines our future. . . . I want to incorporate images that speak about science and technology from the earliest notions of scientific thought and discovery to very contemporary science," Stacey says. "Love Fingers" (see center, opposite page) is among the works she has produced at NCSA.

Her work has been seen in many exhibits and is currently being shown at the Metropolitan Museum of Photography in Tokyo.

Edmond Prakash is a scientific officer at the Computer Science Education and Research Center at the Indian Institute of Science, Bangalore, India. His visit was funded by the United Nations Development Program.

Prakash's work involves studying the human-computer interface and using scalable architectures to help researchers produce scientific visualizations more easily.

Christa Sommerer (from Austria with a background in botany and fine arts) and **Laurent Mignonneau** (from France with a fine and applied arts background) teamed up when they met at the Institut für Neue Medien, Städelschule, Frankfurt, Germany in 1992.

Their work, "Interactive Plant Growing," deals with the sensitive relationship between real plants and human viewers (see left, top and center, this page). Viewers use their hands to initiate and control in real-time 3D plant growth on the screen of a Silicon Graphics workstation. Fine voltage exchanges between plants and viewers are captured by a special interface. These signals control plant algorithms (developed by Mignonneau-Sommerer) that are visualized as virtual plant growth on the screen. ▲

Top to bottom: "Interactive Plant Growing," showing two stages of a sequence, and "Anthroposcope" by Christa Sommerer and Laurent Mignonneau. (Courtesy of the artists)



Detail from "Anthroposcope" (left) by Sommerer and Mignonneau; "Love Fingers" (below left) and detail (below right) by Robyn Stacey. (Courtesy of the artists)



Robyn Stacey

Edmond Prakash

Christa Sommerer

Laurent Mignonneau

(Photos by Tony Baylis, USEO—left and center left; Vincent Jurgens, VEG—center right and right)

NCSA research assistant; and Ed Seidel, NCSA research scientist. *The Fractal Microscope* is an interactive tool designed by the Education Group for exploring the Mandelbrot set and other fractal patterns. Michael South, REU student now in graduate school at Texas Tech, was the primary developer.

A unique aspect of the exhibit was that the demonstrations and other facets of the National MetaCenter could be previewed in a multimedia presentation in NCSA Mosaic. Shown on both an SGI Indigo workstation and an Apple Macintosh, it had top-level links to "Education," "Demonstrations," "Science," and "MetaCenter."

A new feature of NCSA Mosaic for the X Window System, "hotspot mapping," allowed viewers to click on portions of a large image to access the desired information. The URL for seeing the MetaCenter's Supercomputing '93 exhibit

is <http://www.tc.cornell.edu/SC93/SC93Home.html>

Other NCSA involvement in exhibits included networking staff who designed and supported the HIPPI network for SCinet '93. SCinet allowed interactive simulations to be performed on the show floor. Over 50 HIPPI connections were made this year.

HIPPI network staff from NCSA were Randy Butler, team leader; Joseph Godsil; Vijay Rangarajan; Von Welch; and Paul Zawada.

The CAVE

For the second year, the virtual reality CAVE was a major conference attraction with over 1,100 people going through various presentations. UIC's Electronic Visualization Laboratory (EVL) and NCSA collaborated on the project. Enhancements this year included data sonification and interactive, distributed applications using a CM-5. Five Silicon Graphics Crimson systems computed the images on three walls and the floor.

Some NCSA projects involved interactive steering of simulation codes running on a CM-5. They were:

- *The Fluid Universe: Simulations in Astrophysical Fluid Dynamics*—Mike Norman, Greg Bryan, NCSA; Trina Roy, Jon Goldman, UIC.
- *Spacetime Splashes: Catching the Wave of Einstein's Equations*—Ed Seidel, Joan Masso, Dan Weber, NCSA; Jon Goldman, Trina Roy, UIC.

Funding for the CAVE demonstration was provided by ARPA and NSF. Corporate sponsors included Electrohome, Korte Technologies, Silicon Graphics Inc., Systtran Corp., and Thinking Machines Corp.

EVENT

The CAVE is part of the newly established EVENT, the Emerging Virtual Environments National Testbed, another collaboration between NCSA and EVL. This multidisciplinary research effort engages computational scientists and artists in collaborative technology.

"It is scalable from desktop workstations to fully immersive environments, from the mouse to full-tilt motion feedback platforms, and from local to national high-speed access," says Thomas DeFanti, codirector of EVL and visiting associate director for virtual environments at NCSA.

An outreach activity of EVENT is VROOM, a demonstration of about 50 virtual environment projects at the SIGGRAPH '94 conference in Orlando. A national call for participation is bringing together

remote scientists and NCSA/EVL programmers to build virtual environment experiences with emphasis on CAVE technology.

At Supercomputing '95, NCSA/EVL will follow with Super-VROOM to connect virtual environments, gigabit networks, and remote scalable machines. ▲

Milestones continued from page 33

Several NCSA publications won awards in the 21st Annual Technical Publications and Art Competition sponsored by the Chicago chapter of the Society for Technical Communication (STC). **Melissa Johnson** is team leader of the Publications Group.

Winning entries, their personnel, and their standings are as follows: **NCSA data link**, Stephanie Drake and Kenneth Chang, distinguished publication; **NCSA Informational Packet**, Paulette Sancken and Linda Jackson, distinguished art; **access**, Fran Bond and Linda Jackson, excellence art; and **NCSA User Guide Covers**, achievement art, Ginny Hudak-David and Linda Jackson.

NCSA data link went on to the International STC competition to win an award of merit. ▲



Home Page of National MetaCenter online exhibit at Supercomputing '93 using NCSA Mosaic. (Designed by Ingrid Kallick, USEO)

NCSA NETWORKS CHAMPAIGN COUNTY

BY ALAINA KANFER,
APPLICATIONS GROUP

NCSA Director Larry Smarr, in 1993, challenged the Champaign County Chamber of Commerce to steer Champaign County onto the emerging national electronic superhighway [see *access*, Spring 1993].

In response, the chamber appointed an Infrastructure Committee, led by Mike Henneman (Henneman, Raufeisen and Associates Inc.) and Lee O'Neill (Bussey Bank). Subcommittees were charged with (1) identifying potential applications of a high-speed countywide network and (2) investigating the technical options for how sites can connect to the network.

Plans are underway to construct Champaign County Network (CCNet), a network connecting Champaign County residents, organizations, and businesses to each other and to the rest of the world via Internet.

NCSA staff members Larry Smarr, Scott Lathrop, Dan Alpert, Randy Butler, Charlie Catlett, Joseph Hardin, Alaina Kanfer, Melanie Loots, Bill Pottinger, Michael Welge, and Paul Zawada have been working closely with the Chamber of Commerce to make CCNet a reality.

Getting underway

Community, government, and business leaders worked throughout the summer of 1993. Five task forces outlined near- and long-term applications in the following areas: **Community service/government resources/libraries**—information

access for the general public, Geographic Information System with virtual or simulated community component; **Health care**—common formats for patient records, x-rays, and other medical information, electronic delivery of health care to rural areas; **Education**—media centers in the schools, master plan for networking the schools; **Small business**—electronic business directory of services and products; fast interchange of images and large amounts of data among businesses such as design and advertising; **Agribusiness**—agricultural Geographic Information System including roads, parcels, and soil types that can be utilized by local agribusinesses, farming enterprises, and government agencies.

The technical subcommittee members have met with vendors of various media for network connections including cable, telephone, and wireless. A pilot project that involves transmission of data at speeds up to 10Mbps is in the planning stages. Currently, several potential sites in each of the applications areas are investigating the feasibility of a cable connection at their location.

The first stages of the CCNet pilot project are being sponsored by the Champaign County Chamber of Commerce, the Champaign-Urbana Convention and Visitor's Bureau (CUCVB), and the Greater Urbana-Champaign Economic Development Corporation. To oversee development, the Chamber of Commerce established CCNet Inc., a not-for-profit organization.

At the same time that CCNet is being developed, a local Freenet, PrairieNet, is under development to provide free access to electronic mail and information



CCNet screen running on NCSA Mosaic.

(Designed by Ingrid Kallick, USEO)

for all members of the community. PrairieNet presents an interesting, valuable complement to CCNet. While the CCNet project is focused on high-speed, broad bandwidth connections to key sites, the widely used PrairieNet provides relatively low speed (dial-up access) connections to the Internet for any community member on a computer with a modem. PrairieNet is also accessible through the Internet.

Presentations

CCNet's potential advantages to the county—high-speed access to the electronic superhighway—have been presented to the community via the local media.

Ed Scharlau, chairman of Bussey Bank, heralded the information age to over 1,000 community leaders with a live demonstration of possible future electronic services, such as an online business directory and electronic newspapers. Alaina Kanfer demonstrated online information and

encouraged the audience at the Convention and Visitor's Bureau annual dinner to make their information available electronically. The CUCVB exhibit on the Champaign County Home Page is an example.

Online pages were available using NCSA Mosaic due to the efforts of NCSA intern Aaron Kaka, NCSA designer Ingrid Kallick of USEO, and NCSA Publications Group members: Ken Chang, Ginny Hudak-David, Paulette Sancken, and Melissa Johnson, manager.

Community information on NCSA's World Wide Web server is available via the URL for the document: <http://www.ncsa.uiuc.edu/General/ChampaignCty/CountyIcons.html>.

For additional information, contact Scott Lathrop, NCSA community outreach coordinator, by phone at (217) 244-1099; or by email at scott@ncsa.uiuc.edu (Internet). ▲



Artworks at the Beckman Institute—
Left to right: "Pragnanz Series" by
William Carlson (1992); "Untitled" by
Brent Collins (n.d.); and two views of
"Tsunami Rising" by Christian Martens
(1990). (Photos by Thompson-McClellan
Photography)



NEW CONSULTING HOURS

BY GINNY HUDAK-DAVID, NCSA PUBLICATIONS EDITOR,
PUBLICATIONS GROUP

The NCSA National Consulting Office recently announced expanded hours of services. The staff are now available to answer questions from 8:30 a.m. to 6 p.m. (central time).

Users may send electronic mail, call, or visit the office with their questions about the NCSA high-performance computing environment [see *ncta contacts*, page 2].

The hours were changed following an analysis of the locations of the NCSA user base as well as machine usage patterns. According to Consulting Services team leader John Towns, "Our users are located primarily in the eastern and central time zones, so the additional time in the morning should be helpful to those users. The additional hour in the evening will provide timely assistance to our evening users in all time zones and particularly to our mountain [time] and West Coast users."

Towns and the consulting staff will be evaluating users' response to the expanded hours over the next few months. NCSA consultants handle nearly 800 user contacts a month.

NCSA bibliography submission

NCSA relies on our researchers to help us maintain a comprehensive bibliography of work produced on NCSA systems. This bibliographic compilation serves to underscore the impact and scope of the computational work being done at NCSA. We are requesting your assistance in this effort.

We encourage electronic submission of bibliographic information and a project abstract. The form is available on anonymous FTP. Log on to a host at your site that is connected to Internet and running software supporting FTP. Invoke FTP by entering the Internet address of the server: `ftp ftp.ncsa.uiuc.edu` or `ftp 141.142.20.50`. Log on using anonymous for the name and your local login name and address (e.g., `jones@ncsa.uiuc.edu`) for the password. Change to the `/ncsapubs/ResBiblio` subdirectory. Enter `get biblio.form` to transfer the form (ASCII). Complete the requested information and submit the file with the abstract to the electronic mail address below.

If you choose, you may complete this form in hard copy and submit it with a project abstract and, if desired, a copy of your publication to the address given below.

This is an ongoing effort, so please submit materials as they are published or presented. Thank you.

Submitting author's name	Phone	email address
Institution		
Address		
City	State	Zip

The format for listing publications is: last name, first name, first name last name, and first name last name. Title of publication. Journal name, volume number, pages (year). For example: Smith, Jane, Ross Jones, and Alice Brown. Adaptive inverse dynamics control of robots. *Science*, 4, 33-35 (1993)

Author name(s) as shown on the publication
Title
Publication title (e.g. <i>Biochemistry</i> , <i>Science</i>), volume number, page reference, year

Required: NCSA account number (ex: abc) or NCSA grant number (ex: AST910367N): _____

Required: NSF Field of Science (ex: 417): _____

Please check category of your submission:

- | | | | | |
|--|---------------------------------------|------------------------------------|---|--|
| ☐ journal | ☐ magazine | ☐ preprint | ☐ technical report | ☐ journal cover |
| ☐ presentation/proceeding | ☐ dissertation | ☐ thesis | ☐ book/chapter | ☐ video |
| ☐ submitted | ☐ in press | ☐ published | | |

Abstract: Provide an online abstract of no more than 150 words to biblio@ncsa.uiuc.edu (ASCII format; do not embed equations in your ASCII file). Please include the title of your work for cross reference.

Submit to: Research Bibliography
NCSA/UIUC
152 Computing Applications Building
605 East Springfield Avenue
Champaign, IL 61820-5518

email: biblio@ncsa.uiuc.edu
phone: (217) 244-5359



abbreviations

ARPA	Advanced Research Projects Agency
CRI	Cray Research Inc.
HPCC	High Performance Computing and Communications
NASA	National Aeronautics and Space Administration
NCAR	National Center for Atmospheric Research
NCSA	National Center for Supercomputing Applications
NII	National Information Infrastructure
NOAA	National Oceanic and Atmospheric Administration
NRAO	National Radio Astronomy Observatory
NSF	National Science Foundation
TMC	Thinking Machines Corp.
UIC	University of Illinois at Chicago
UIUC	University of Illinois at Urbana-Champaign
URL	Uniform Resource Locator

documentation orders

Articles in this *access* may refer to items that are available through the NCSA *Technical Resources Catalog*. To receive a copy of the catalog, send your request to Orders for Publication, NCSA Software, and Multimedia [see ncsa contacts, page 2].

accessing NCSA's servers

Many NCSA publications (e.g., calendar of events, user guides, *access*, technical reports) as well as software are available via the Internet on one of three NCSA servers: anonymous FTP, Gopher, or the World Wide Web. If you are connected to the Internet, we encourage you to take advantage of the easy-to-use servers to copy or view files.

Anonymous FTP IP address: `ftp.ncsa.uiuc.edu` (141.142.20.50)

Gopher server IP address: `gopher.ncsa.uiuc.edu`

World Wide Web IP address: `www.ncsa.uiuc.edu`

NCSA WWW Home Page: `http://www.ncsa.uiuc.edu/General/NCSAHome.html`

NOTE: References in *access* to a World Wide Web URL (Uniform Resource Locator) refer to the server address and file location information used by NCSA Mosaic software to retrieve documents.

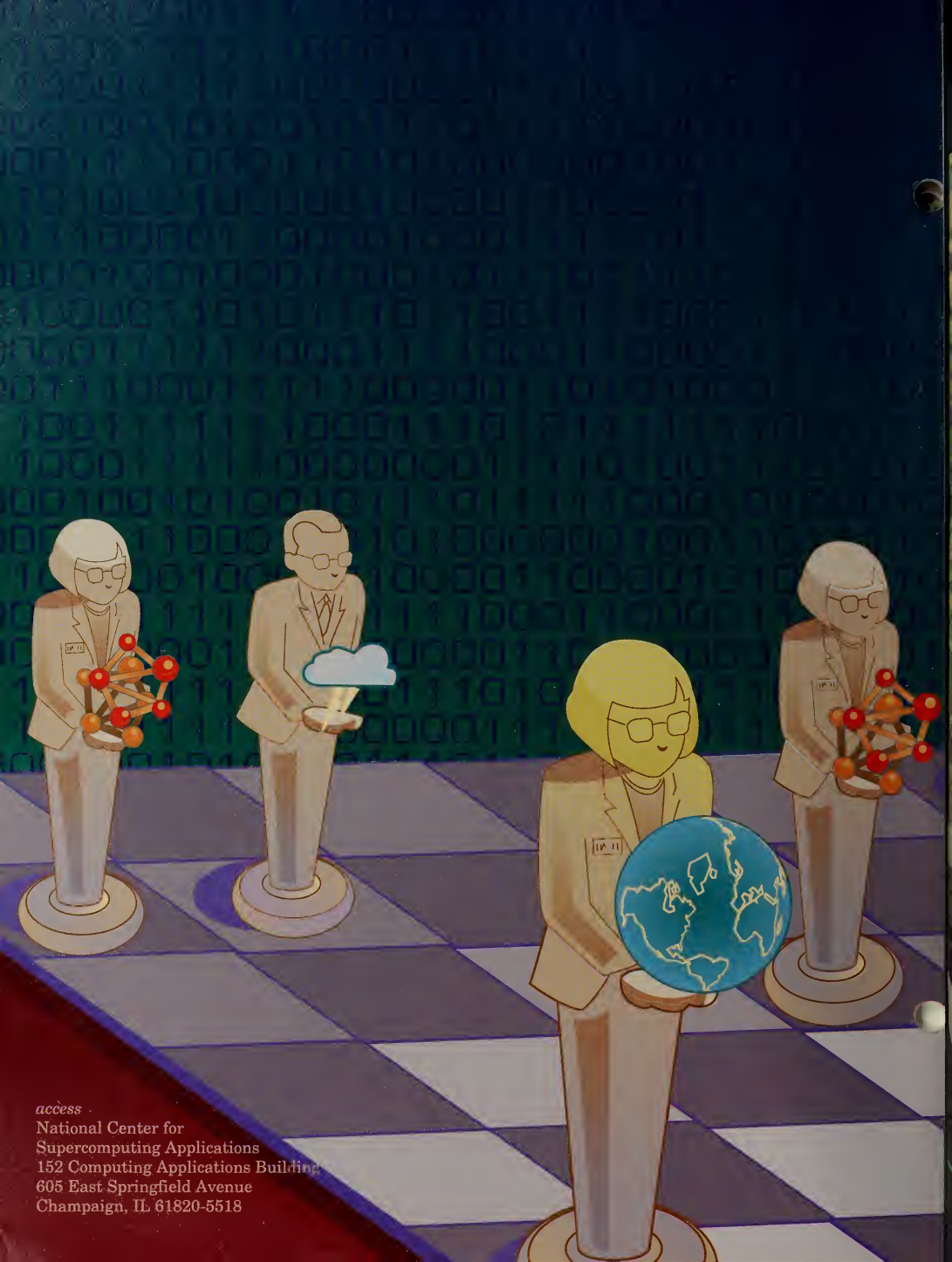
If you have any questions about accessing the servers, contact your local system administrator or network expert. Instructions for accessing the anonymous FTP server follow.

downloading from anonymous FTP server

A number of NCSA publications are installed on the NCSA anonymous FTP server. If you are connected to Internet, you can download NCSA publications by following the procedures below. If you have any questions regarding the connection or procedure, consult your local system administrator or network expert.

1. Log on to a host at your site that is connected to Internet and running software supporting the FTP command.
2. Invoke FTP by entering the Internet address of the server: `ftp ftp.ncsa.uiuc.edu` or `ftp 141.142.20.50`
3. Log on using `anonymous` for the name.
4. Enter your local login name and address (e.g., `smith@ncsa.uiuc.edu`) for the password.
5. Enter `get README.FIRST` to transfer the instructions file (ASCII) to your local host.
6. Enter `quit` to exit FTP and return to your local host.
7. The NCSA publications are located in the `ncsapubs` directory.

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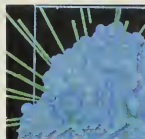
25 book review



Cover: Virtual environments for investigating science and engineering projects, one of NCSA's major technology directions, is the subject of this issue. Symbols from science and fine art represent the melding of these two knowledge bases that are needed in the creation of interactive, immersive technologies.

Cover produced on a Macintosh IIci using Adobe Photoshop, Adobe Dimensions, Aldus FreeHand, and a UMAX UC630 scanner. (Concept and illustration, John Havlik; concept and research, Fran Bond)

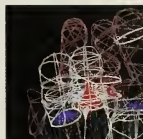
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An apology

In the Book Review of the Spring 1994 *access*, incorrect URLs for locating *Wired* and *GNN Magazine* on the World Wide Web were given. Correct URLs are: <http://www.wired.com/> (*Wired*) and <http://gnn.com/> (*GNN Magazine*). We regret the error.

Summer 1994

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CoVis

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NCSA bibliography submission

NCSA relies on our researchers to help us maintain a comprehensive bibliography of work produced on NCSA systems. This bibliographic compilation serves to underscore the impact and scope of the computational work being done at NCSA. We are requesting your assistance in this effort.

We encourage electronic submission of bibliographic information and a project abstract. The form is available on anonymous ftp. Log on to a host at your site that is connected to Internet and running software supporting FTP. Invoke FTP by entering the Internet address of the server: **ftp ftp.ncsa.uiuc.edu** or **ftp 141.142.3.135**. Log on using anonymous for the name and your local login name and address (e.g., jones@ncsa.uiuc.edu) for the password. Change to the /ncsapubs/ResBiblio subdirectory. Enter **get biblio.form** to transfer the form (ASCII). Complete the requested information and submit the file with the abstract to the electronic mail address below.

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VIRTUALLY EXPERIENCING SCIENCE

Have you wished you could enter the lush landscape of a stunningly visual film—the Golden Valley of the recent “Shadowlands,” for example—as Mia Farrow’s character in the “Purple Rose of Cairo” by Woody Allen did? Or maybe when you first began using a microscope to view infinitesimal protozoa in biology lab you wanted the chance to enter their world and get an even closer look.

VROOM, a virtual reality room using CAVE (Cave Automatic Virtual Environment) state-of-the-art facilities, can satisfy both those whims. This immersive technology puts researchers right in the middle of molecular dynamics, under the sea’s surface, and into other natural phenomena. Beginning on page 4, you will explore this innovative scientific research medium in “A virtual environments toolset driven by science.” Users of this interface introduce their findings on pages 6 and 7 and 9 through 14. Whether or not there is “Truth in science imagery” is discussed on page 15.

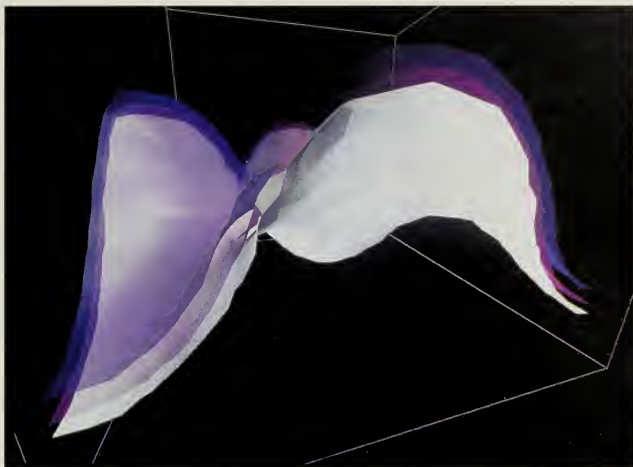
Through the use of ZEUS codes developed at NCSA, Astronomer Mordecai-Mark Mac Low of UIUC and the University of Chicago, simulates the galactic event of this summer—a comet crashing into Jupiter (see page 17). The developer of those codes, NCSA Research Scientist Mike Norman, recently announced the running of the world’s largest cosmology simulation on NCSA’s CM-5 (see page 27).

Other articles include the winning of the third NCSA Industrial Grand Challenge Award by two researchers from FMC Corporation (page 18) and collaborative visualization in classrooms utilizing NCSA Mosaic (page 20). Several articles feature uses and awards for NCSA Mosaic (pages 19, 22, 23, and 28).

Multimedia users and developers will be especially interested in Kenneth Chang’s book review on page 25.

New platforms entering NCSA’s computational environment and older platforms being retired are announced in Director Larry Smarr’s letter on page 24. Watch for more information about these changes in the next issue of *access*.

—Fran Bond, Editor



Still from *The Fluid Universe: Rayleigh-Taylor Instability in Fluid Flow*, Greg Bryan and Mike Norman, NCSA; Trina Roy and Jon Goldman, EVL/UIC. An interactive simulation showing what happens when a heavier fluid lies on top of a lighter one.

A virtual environments

by Jarrett Cohen, Senior Publications Specialist, NASA/Goddard

"Human brains are not particularly good at navigating in two dimensions," says Jim Bower, a Caltech biologist using virtual reality to study the brain.

"We have a lot more sophisticated power to deal with three dimensions. . . . You can readily navigate to where you want [and do so] more powerfully, precisely. 2D was an invention we were forced to deal with because of previously limited technology."

Bower stresses that "it basically comes down to what kind of a world the nervous system was designed to work in, which is basically the one we live in."

The intuitive nature of 3D navigation is the strength of virtual environments, which—together with scalable metacomputing and cyberspace tools—are the major technology directions at NCSA.

VEG

NCSA's Virtual Environments Group (VEG) seeks to make these interactive, immersive technologies usable for investigating problems in science and engineering.

They are undertaking this task in collaboration with UIC's Electronic Visualization Laboratory (EVL). EVL Director Thomas DeFanti considers

his appointment as NCSA visiting associate director for Virtual Environments a formalization of the EVL-NCSA collaboration ongoing since 1986.

"It is also much like the National MetaCenter in that it draws on the strengths of each collaborator," he says. "NCSA brings supercomputing and networking expertise, while EVL brings interactive graphics expertise."

NCSA faculty, staff, and students in VEG, some of whom work in other groups as well, include Ulrike Axen, Polly Baker, Robin Bargar, Tony Baylis, Donna Cox, Alan Craig, Kelly Fitz, George Francis, Ping Fu, Camille Goudeseune, Chris Hartman, Vincent Jurgens, Mark Lumos, Bill Sherman, Jeff Terstriep, Mark Washburn, Daniel Weber, and Erik Wesselak.

EVL

EVL was founded in 1973 by DeFanti, UIC professor of electrical engineering and computer science, and Director Dan Sandin, professor of art and design. From the beginning the lab has reflected their backgrounds, effecting a "unique interdisciplinary blend of engineering, science, and art," says EVL Associate Director Maxine Brown.

EVL currently has six full-time faculty/staff and 55 graduate students. EVL faculty and staff members include DeFanti, Sandin, Brown, Gary Lindahl, Dana Plepys, and Maggie Rawlings.

Early contributions to computer graphics included performances with real-time graphics accompanied by music and the use of its hardware and software for creating the computer animation of the Death Star "schematic" for the first *Star Wars*. In 1976, based on an idea by colleague Rich Sayre, DeFanti and Sandin developed an inexpensive, lightweight glove to monitor hand movements; the Sayre Glove provided an effective method for multidimensional control, such as mimicking a set of



Navigator's head gear with location sensor. (Photo by Thompson-McClellan Photography)

toolset driven by science

Space Flight Center; former NCSA Staff Associate, Director's Office

sliders. Projects in the 1970s through mid-1980s centered on video game technology, real-time computer animation on microcomputers, and interactive multimedia installations.

"In the late 1980s, the lab began focusing on scientific visualization, developing and providing tools and techniques for research scientists and engineers," Brown says. "Continuing these efforts, EVL is now applying virtual environments to scientific computing."

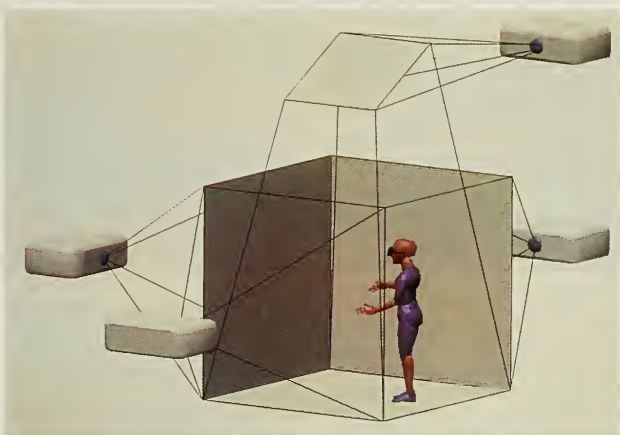
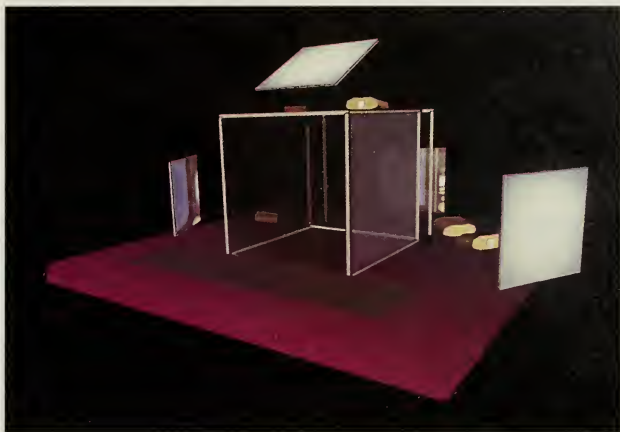
The CAVE

The primary interface that VEG is exploring is the CAVE, short for Cave Automatic Virtual Environment. The CAVE was first conceived of by DeFanti and Sandin in the spring of 1991 and implemented by Ph.D. student Carolina Cruz-Neira and others at EVL.

In the CAVE, high-resolution stereoscopic images are generated by a multiprocessor Silicon Graphics workstation or multiple workstations and rear-projected onto several walls and front-projected onto the floor, using mirrors to fold the optics. Participants wear stereo glasses to view the images in 3D. A head-tracking device is affixed to the glasses worn by the navigator, and a hand-tracking device with input controls—called the "wand"—is used to interface with the environment.

"The reason it works very well is because, unlike a head-mounted display, the whole world does not have to turn when you turn your head," DeFanti explains. "The CAVE is like the real world. The perspective changes subtly, but that is a much less radical phenomenon than changing the world."

The capability of sharing findings with others, however, is the most significant benefit of the interface, he says. "It preserves the teacher-student/salesman-customer relationship."



The CAVE is a multiperson, room-sized, high-resolution, 3D video and audio environment. Graphics are rear projected in stereo onto three walls and the floor and viewed with stereo glasses. As a viewer wearing a location sensor moves within its display boundaries, the correct perspective and stereo projections of the environment are updated. Above ©1993 Milana Huang, EVL/UIC; below ©1992 Lewis Siegel and Kathy O'Keefe, EVL/UIC (Courtesy of EVL/UIC)

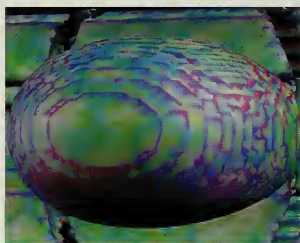
Getting Physical in Four Dimensions

Sessions—Daniel Sandin, Joanna Mason, and Milana Huang, EVL/UIC; Lou Kauffman, Dept. of Mathematics, Statistics, & Computer Science, UIC; George Francis, NCSA/UIUC. This application's goal is to provide a more intuitive understanding of hyperspace, enabling VROOM participants to interact in 4D with objects.

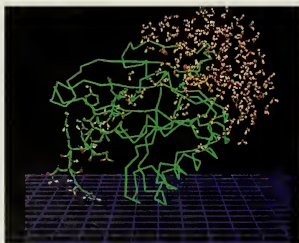
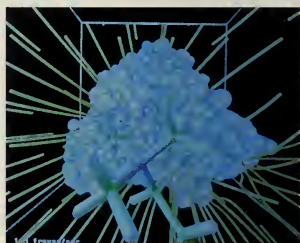


Evolution of Behavior in a Simulated Environment

—Michael Papka, Sumit Das, and Terry Franguiadakia, EVL/UIC. Virtual reality enables CAVE users to interact with various *animats*, virtual animals exhibiting behaviors similar to animals in nature, which is based on Artificial Life, the study of living organisms via artificial means.



Acetylcholinesterase: Nature's Vacuum Cleaner—Richard Gillilan and Daniel Ripoli, CTC. By literally moving into the *acetylcholinesterase* enzyme along a route taken by neurotransmitter molecules, researchers can examine electrostatic fields and other aspects of enzyme activity.



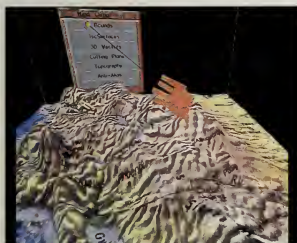
Interactive Molecular Modeling Using Real-time Molecular Dynamics Simulations and Virtual Reality Computer Graphics—Paul Bash, Center for Mechanistic Biology & Biotechnology, ANL; George Lent and John Rowlan, Mathematics & Computer Science Div., ANL; Carolina Cruz-Neira, EVL/UIC. This project shows how drug designers can interact with molecular models on the visual and aural planes via VR by demonstrating the docking of a drug molecule to its molecular receptor.

Virtual Director—Marcus Thiébaux, EVL/UIC; Donna Cox, NCSA/UIUC, and Robert Patterson, NCSA. This application, which can be used for varied 3D image settings and scientific datasets, demonstrates a virtual reality method for controlling camera motion in animations and an astronomical simulation of colliding galaxies. VR provides a real-time interface for camera motion viewing, recording, and playback.

3D Terminal Viewer (3DTV)—William Myers, Bob Barron, Gerry Wiener, and Zhongqi Jing, Research Applications Program, NCAR; Don Middleton and John Clyne, Scientific Computing Div., NCAR. This application was developed to study the value of real-time 3D visualization of weather hazards like microbursts, wind gust fronts, and regions of heavy precipitation for the aviation community.

(Images Courtesy of EVL/UIC)

Visualization of Climate Data over the Western United States—Peter Kochevar, DEC/SDSC; Michael Bailey, Michael Kelley, and Jim McLeod, SDSC. Output from a regional climate model for the western U.S. utilizes the virtual environment to help climatologists better understand energy transport in the atmosphere.

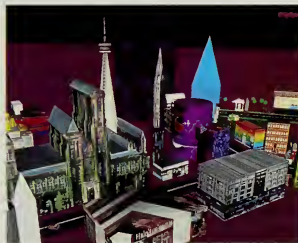


3D Hydrodynamic Model of the Heart—Joel Welling and Grace Giras, PSC; Charles Peskin and David McQueen, Courant Institute, NY. A computational model of the heart is used in this project that is investigating VR applications in biomedical research. In this study, the heart is treated as a set of fibers immersed in fluid—responsive to fluid and tensile forces.



Virtual Breadcrumbs: A Tracking Tool for Biological Imaging—Clinton Potter and George Baxter, NCSA/UIUC; Andrew Belmont and John Pixton, UIUC; Rachael Brady and Patrick Moran, NCSA; Bridget Carragher, Beckman Institute/UIUC. An immersive virtual environment tracking tool for tracking complex biological structures is how Virtual Breadcrumbs can be described. The tool is demonstrated with several biological and medical datasets in the CAVE, which provides a unique environment for 3D image analysis.

CitySpace—Coco Conn and Zane Vella, Internet Tours; Jim Damiano, Spatial Relations; Jim Thompson, Smallworks; Chris Cederwell, EVL/UIUC. This educational networking project is designed for self-managing groups of students, mentors, teachers, and resource administrators. Participants from around the world are invited to build a virtual city model of 3D objects and images.



The CAVE may be used both to explore precomputed datasets and to interactively steer supercomputer simulations.

The first CAVE was built at EVL and publicly displayed at SIGGRAPH 92 as part of Showcase [see access, May–June; July–September, 1992]. There were subsequent demonstrations at Supercomputing '92 and '93, with a 64-node CM-5 available onsite for simulations at the latter [see access, Spring 1994].

NCSA's CAVE measures 10 x 10 x 9 feet and is housed in a specially modified room at the Beckman Institute for Advanced Science and Technology. Echoing the "Holodeck" on *Star Trek: The Next Generation*, a grid crisscrosses the ceiling and walls near the CAVE. Images appear on two or three walls and the floor; sound emanates from four speakers in the corners, providing ambience and data-driven feedback.

The images are computed by a four-processor SGI Onyx system with three Reality Engines. The Onyx connects via HIPPI to NCSA's supercomputers, of which the CM-5 and SGI Challenge are being emphasized for virtual environments.

Sound is produced by the Ensoniq ASR-10 synthesizer and the Yamaha 990 signal processor. The demand for virtual sound cannot be met by existing commercial products; however, NCSA is developing interactive sound synthesis techniques using an SGI Indigo as a dedicated server, says Robin Bargar, who is coordinating audio development. Sound is digitally placed in three dimensions utilizing an MX-16 system similar to those used by Lucasfilm. [See page 12 for more details about sonification in virtual reality (VR).]

Other CAVEs have been built at the ARPA Enterprise (Arlington, VA) and the Argonne National Laboratory (Argonne, IL, near Chicago).

EVENT

These R&D activities are occurring in the context of EVENT, the Emerging Virtual Environments National Test-bed [see access, Spring 1994], the goal of which is "to provide a complete virtual environments toolset driven by science," DeFanti says.

The areas of emphasis are hardware integration and development, system software, investigation of different modes of interaction/navigation, and outreach. (For a more complete list of such efforts, see CAVE research, page 8.)

"It is now very much like the early days of visualization, where everything was custom," DeFanti says. "EVENT is unique in that it has application focus to both HPCC and NII. The awesome level of resources that we are throwing at it—BLANCA [the gigabit network testbed], high-speed supercomputers, and high-end Silicon Graphics workstations—also make EVENT unique."

VROOM and SuperVROOM

Major outreach components of EVENT are VROOM (SIGGRAPH 94) and SuperVROOM (Supercomputing '95), demonstrating "computational science/engineering and scientific visualization in virtual environments," says Brown, VROOM cochair with DeFanti.

VROOM, virtual reality room, involves public display of applications in three CAVEs and about five Fakespace Inc. BOOMs (Binocular Omni-Oriented Monitors) at SIGGRAPH 94 in Orlando, with several onsite supercomputers. Researchers based internationally will work with EVL, NCSA, and Argonne National Laboratory (ANL) to develop VR projects. NSF, ARPA, DoE, and NASA are providing funding.

Thirty institutions submitted 66 proposals. Forty-three projects were chosen by a jury composed of Steve Bryson, NASA Ames Research Center; James George, Mesa Graphics; Larry Smarr, NCSA; and Rick Stevens, ANL. (See page 10.)

Fields represented in VROOM include atmospheric and ocean sciences, astrophysics, biology, fluid dynamics, manufacturing and industrial design, and mathematics.

CAVEviewer

Participants will use CAVEviewer, a tool that simulates CAVE applications on SGI workstations, via NCSA Mosaic for development work at their home institutions. "Final adaptation to the actual CAVE environment will be conducted 'on-location' at the vari-

ous CAVE sites," says Dana Plepys, EVL documentation project manager. The CAVEviewer will also be used as a presentation tool at VROOM. "Further exploration of VR projects will be made possible through multimedia presentations [that] incorporate the CAVEviewer for real-time interaction with CAVE applications at the desktop," Plepys says. VROOM documentation will be available following SIGGRAPH 94 via the Internet using NCSA Mosaic.

Part of Supercomputing '95 in San Diego, SuperVROOM will move to the next level, employing several gigabit network testbeds for interactive steering of simulations on near-teraflop machines.

"I would like to get as close to a peak teraflop as we can, the equivalent of 100,000 normal workstations," DeFanti says. "The basic idea is to extend VROOM... to groups across the country working on the same problem."

This building of collaborative teams will be the major contribution of these public displays, he stresses.

Virtual continued on page 26



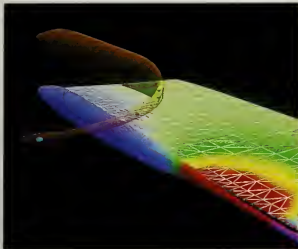
"Unlike workstation graphics, where you are on the outside looking in, in the CAVE you are on the inside looking out," says EVL Director Thomas DeFanti, who is NCSA's visiting associate director for Virtual Environments. (Courtesy of DeFanti)

Look for the URL for viewing VROOM in the next issue of access.

CAVE research

Current EVL and NCSA efforts using the CAVE include:

- a scalable workstation (developing the necessary hardware and software to make the CAVE an intelligent user interface to supercomputers, superworkstations, massive data stores, or other VR devices, over high-speed networks)
- new methodologies for human/computer interaction and navigation (from new 3D graphical icons to voice and gesture recognition)
- virtual environment documentation (scripting, capture, edit, and replay tools)
- virtual environment library and emulators (a core VR library that works with any VR device and interfaces to any graphics library or toolkit)
- digital libraries (the ability to access massive datasets from the CAVE and the ability to store VR-related files: models, sounds, programs, etc.)
- sound/sonification tools (an audio library and prototype tools for use with scientific data)
- visualization techniques applied to virtual environments (advanced rendering techniques)
- augmented reality (the combination of live action with computer-generated effects)
- CAVE development (for example, larger CAVEs, desktop CAVEs, HDTV CAVEs)
- virtual environment hardware (testing new equipment for better resolution, brightness, and/or speed)
- virtual environment tools (scientific tools for problem solving)
- outreach (knowledge transfer to other researchers and practitioners through demonstrations at professional conferences)



Phase and Amplitude Maps of the Electric Organ Discharge of the Weakly Electric Fish, *Apteronotus leptorhynchus*—Jim Bower, Chris Assad, and Brian Rasnow, Computational and Neural Systems Program, Caltech; Jason Leigh and Thomas DeFanti, EVL/UIC. (Courtesy of EVL/UIC)

Aimed at probing the workings of the brain, Jim Bower's work at Caltech involves three areas of investigation: behavior analysis, electrophysiology, and computer models.

"All [of these] involve a tremendous amount of data and looking for patterns," says Bower, an associate professor of biology. "The best pattern recognizer is our own nervous system. The more sophisticated we are in exposing [it] to those patterns, the more likely we will understand what's going on."

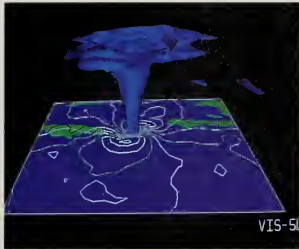
Previous efforts in VR have involved visualizing simulations of many thousands of neurons and detailed simulations of neurons in the CAVE. The project being shown in VROOM involves weakly electric fish, whose "vision is based on changes in electric fields induced by objects."

"As a mammal, I have no experience with electrical sense," Bower says. "Using VR in the lab, we can try to get some sort of a feel for what electric sense is like."

"We simulate the electric fields on fishes' skin and see how they change," he continues. "These studies generate insight and intuition about a sensory system that we are not familiar with. We're using VR to understand the reality of another animal."

The Caltech team has run simulations on the institute's Intel Touchstone Delta system and is now moving their simulations to the new Intel Paragon. They have also used networked workstations running in parallel.

"With simulations of the brain, VR provides us with a way to use the full pattern capacity of the nervous system," Bower says. "In the fish case, it is the only way to do it."



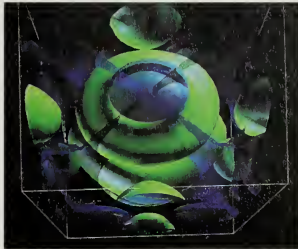
The SIGGRAPH 94 Daily Weather Forecast—Bill Hibbard, Brian Paul, and André Battaola, Space Science and Engineering Center, U. of Wisconsin-Madison; Gregory Tripoli and Peter Pokrandt, Dept. of Atmospheric & Oceanic Sciences, U. of Wisconsin-Madison; Steve Cohen, EVL/UIC. (Courtesy of Hibbard)

The Wisconsin research team has developed VIS-5D (Visualization of 5D Datasets), an interactive visualization system that creates a "virtual earth environment." Users interact with a small graphical Earth, either an ocean or an atmosphere, behind the workstation screen. The CAVE allows the team to adapt the application to an immersive environment for the first time. (The image shown is in VIS-5D applied to Hurricane Gilbert.)

"This is a takeoff on something we have done at the American Meteorological Society meeting," says Bill Hibbard, researcher at the center. "We ran a weather model in Madison every night; it was a two-day forecast of the U.S. We brought the forecast results to the booth over the Internet and showed it on the workstation. Attendees could use it to get a clear idea of weather for their flights."

Hibbard says that the weather forecast is usually very general. What people really want to know is if it is going to be raining at 3 p.m. in their hometowns, for instance.

"This system lets people ask these very specific questions," Hibbard says. "It is high-resolution in both space and time."



Spacetime Splashes: Catching the Wave of Einstein's Equations—Ed Seidel, Joan Masso, Paul Walker, and Dan Weber, NCSA/UIUC; Jon Goldman and Trina Roy, EVL/UIC. (Courtesy of EVL/UIC)

Since last summer, Ed Seidel and his NCSA colleagues have been using the CAVE to look at the evolution of gravitational waves in a 3D spacetime.

"If you have 1 million zones in 3D, it is very difficult to understand the evolution of the system on a 2D screen with 2D graphics," explains Seidel, research scientist in gravitation and team leader of the Gravitation Group. "The CAVE allows us to go in and out of the system in a 3D, intuitive way and allows us to identify features—which might be just behind us—that we might overlook in a traditional graphics environment."

Beyond their initial Supercomputing '93 effort, Seidel would like to add several features to their CAVE software. These include interactive control of the simulation code on the CM-5 and extraction of quantitative information—something Seidel feels has been lacking in scientific visualization.

"You don't have the capability to analyze things quantitatively," he says. "We want to get this back into visualization and into the CAVE—put this question of measures into the visualization software."

VROOM projects

Project titles/contacts/sponsoring organizations for VROOM projects follow:

Sounds from Chaos in Chua's Circuit—Robin Bargar (NCSA)

The Fluid Universe: Rayleigh-Taylor Instability in Fluid Flow—Greg Bryan (NCSA)

Post-Euclidean Walkabout—George Francis (NCSA)

Stepping into Alpha Shapes—Ping Fu (NCSA)

Virtual Breadcrumbs: A Tracking Tool for Biological Imaging—Clinton Potter (NCSA)

Spacetime Splashes: Catching the Wave of Einstein's Equations—Ed Seidel (NCSA)

Molecular Recognition in Protein-Protein Association—Shankar Subramaniam (NCSA)

The Development of Tornadoes with Storms and Along Gust Fronts—Robert Wilhelmson (NCSA)

Using Virtual Reality for Machine Design—Dee Chapman (Caterpillar Inc., NCSA)

DETOUR: Brain Deconstruction Ahead—Rita Addison (Independent)

Interactive Molecular Modeling Using Real-time Molecular Dynamics Simulations and Virtual Reality Computer Graphics—Paul Bash (Argonne)

Simulation of a Grinding Process in Virtual Reality—Thomas Canfield (Argonne)

Interactive Adaptive Mesh Refinement—Lori Freitag (Argonne)

Visualization of Casting Process in Foundries—Robert Schmitt (Argonne)

Distributed Interactive Molecular Dynamics—Klaus Schulten (Beckman Institute, UIUC)

RealEyes: A System for Visualizing Very Large Physical Structures—Henry Sowizral (Boeing)

Phase and Amplitude Maps of the Electric Organ Discharge of the Weakly Electric Fish, Apteronotus Leptorhynchus (Brown Ghost)—James Bower (Caltech)

Acetylcholinesterase: Nature's Vacuum Cleaner—Richard Gillilan (CTC)

Visualization of Climate Data over the Western United States—Peter Kochevar (DEC, SDSC)

Simulation of Light and Sound Distribution in an Environment—Peter Astheimer (Fraunhofer Institute)

Knotted Spheres in the Fourth Dimension—Andrew Hanson (Indiana U.)

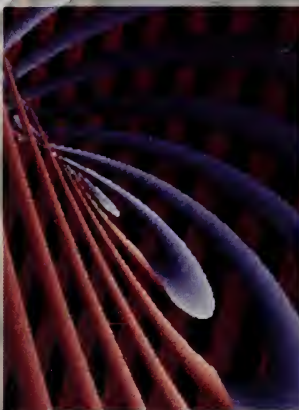
The Onset of Turbulence in a Shear Flow over a Flat Plate—David Banks (Institute for Computer Applications in Science & Engineering)

CitySpace—Coco Conn (Internet Tours)

The Virtual Windtunnel—Steve Bryson (NASA Ames)

3D Terminal Viewer (3DTV)—William Myers (NCAR)

Scientific Visualization of Gyrofluid Tokamak Turbulence Simulation—Gary Kerbel (Nat'l. Energy Research Supercomputer Center)



A Walk through Chesapeake Bay—Eileen Hofmann (Old Dominion U.)

3D Hydrodynamic Model of the Heart—Joel Welling (PSC)

MUSE: Multidimensional User-Oriented, Synthetic Environment—Creve Maples (Sandia)

Real-time Graphics Techniques Using IRIS Performer—Jim Helman (SGI)

Virtual Exploration of a Florida Thunderstorm Using the SciAn Visualization Package—Eric Pepke (Supercomputer Computations Research Institute)

Stepping into Reality—Edmund Baur (U.S. Army Research Lab)

Parallel Real-time Radiosity—Jon Goldman (UIC)

The Virtual Eye—Paul Neumann (UIC)

JASON Interactive Mapper—Dave Pape (UIC)

Evolution of Behavior in a Simulated Environment—Michael Papka (UIC)

Getting Physical in Four Dimensions—Daniel Sandin (UIC)

Virtual Director—Marcus Thiébaux (UIC)

Topological Surface Deformation—Alan Verlo (UIC)

Virtual Reality for Parallel Computer System Performance Analysis—Dan Reed (UIUC)

Computational Modeling for Crashworthiness of Electric Vehicles Using Nonlinear Finite Element Methods—Roger Engelmann (USC)

The SIGGRAPH 94 Daily Weather Forecast—Bill Hibbard (U. of Wisconsin-Madison)

The SANDBOX: Scientists Accessing Necessary Data Based on eXperimentation—Andrew Johnson (Wayne St. U.)

Still from *Getting Physical in Four Dimensions*, Daniel Sandin, Joanna Mason, and Milana Huang, EVL/UIC; Lou Kauffman, Dept. of Mathematics, Statistics, & Computer Science, UIC; George Francis, NCSA/UIUC. (Courtesy of EVL/UIC)

Step into α by Ginny Hudak-David, NCSA Publications Editor, Publications Group

A finite set of points in 3D space and a real parameter α uniquely define a simplicial complex, also called the alpha complex of the points. An alpha shape is the geometric object defined as the union of the elements in the complex. In 1983, a mathematically rigorous definition of alpha shapes was first introduced by Waterman Award winning Professor of Computer Science Herbert Edelsbrunner, UIUC. The first notion of alpha shapes is the 2D analog of the spatial notion described below.

Alpha shapes formalize the intuitive notion of shape. For varying parameter alpha, it ranges from crude to fine in complexity. The most crude shape is a convex hull, which is obtained for very large values of alpha. As alpha decreases, the shape shrinks and develops cavities that may join to form tunnels and voids.

A related notion is the space filling diagram, which is used in biology and chemistry to represent molecular structures. The space filling diagram is the union of balls centered at the points, and it has a geometrically dual alpha complex.

Alpha Shapes Version 2.0 software—from NCSA's Software Development Group (SDG)—is used in several demonstrations in NCSA's CAVE called *Stepping into Alpha Shapes*. It provides three utilities to visualize a 3D simplicial complex, such as a *Delaunay triangulation*. Named for the Russian Geometer Boris Delaunay, the triangulation "is uniquely defined for a given point set, and it maximizes minimum angles," says SDG Research Programmer Ping Fu, who adds that it is used often in grid generation, modeling, and graphics.

First, by choosing different values of alpha, different subcomplexes are seen providing insight into the detailed structure of the complex. Second, the simulation of a continuous explosion separates the vertices, edges, triangles, and tetrahedra and thus permits visual inspection of the way these pieces fit together. Third, a directed wave can

be propagated through the complex to highlight how it is connected and where the holes are. The wave is a 2D front that advances through the entire complex.

An auditory experience of the complex is made possible through real-time sound synthesis based on the advancing wave. Different features of the wave are mapped to different sound parameters.

The goal is to explore the complex with meaningful auditory and visual cues.

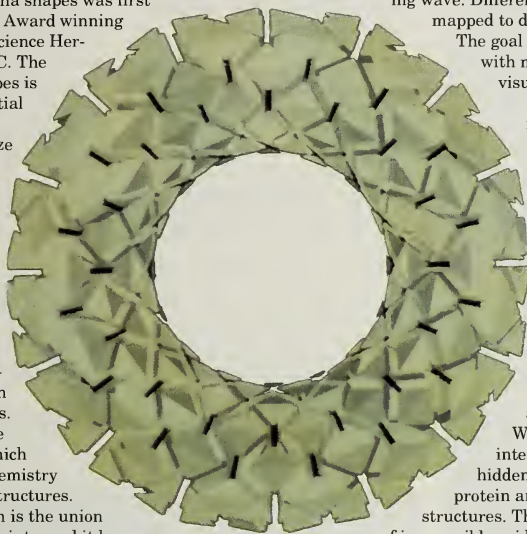
The virtual reality environment of the CAVE and the geometric structure provided by the alpha shape software complement each other. The software constructs an object with detailed features on the outside and inside. The CAVE allows an immersive visual and auditory inspection of the features of the object that is difficult to achieve on a 2D computer screen.

With the VR environment interface, a biologist can enter hidden regions (voids) within a protein and explore their detailed structures. This is relevant to the study of inaccessible voids and protein folding.

Cosmologists say that as the universe expands, galaxies are clustered into sheet-like structures, surrounding large voids. To explore this global cosmological structure, alpha shapes are an exciting new tool when coupled to numerical simulation and virtual reality visualization. The full spectrum of alpha shapes promises to be useful in this study.

Alpha Shapes Version 2.0 software for SGI workstations is available on the NCSA anonymous FTP server (see inside back cover). The CAVE demonstration using the software was developed by Ping Fu and Gilles Bourhis (SDG), and Robin Bargar, (VEG), NCSA; Herbert Edelsbrunner and Ulrike Axen, UIUC Department of Computer Science; and Insook Choi, UIUC School of Music and Department of Computer Science. ▲

NOTE: Ping Fu contributed to this article.

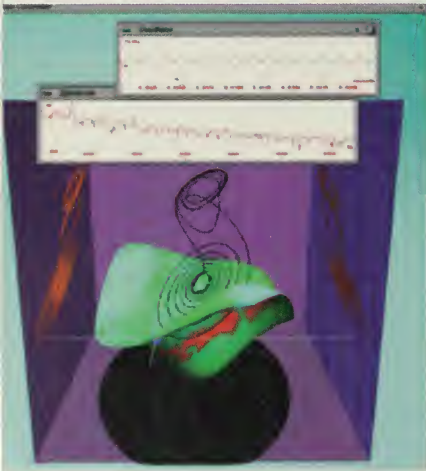


Still from *Stepping into Alpha Shapes*, Ping Fu, Robin Bargar, Gilles Bourhis, and Camille Goudeseune, NCSA; Herbert Edelsbrunner, Ulrike Axen, and Insook Choi, UIUC.
(Courtesy of EVL/UIUC)

Many visitors to SIGGRAPH 94 would agree that chaos is a fitting term to describe the mayhem associated with the week-long event. In addition to the chaos of SIGGRAPH, visitors lucky enough to get into the CAVE to see and, more importantly, hear the virtual reality model *Sounds from Chaos in Chua's Circuit*, will experience mathematical chaos in the virtual environment.

Open your ears to the sounds of chaos

by Victor Ryckaert, NCSA Student Intern



A manifold surface for navigating the control space of Chua's circuit. Both input circuit parameter values and output signal are displayed in the same space. This interface was designed by Insook Choi for exploring chaotic systems and generating musical signals. (Courtesy of Bargar and the Audio Development Group)

Innovators at NCSA have created a graphical interface that allows users to hear the chaos created in Chua's circuit and alter the sounds it produces. This opens the door for two seemingly unrelated disciplines to come together—music and science.

"We are using sound to enhance scientists' experience by inventing ways that data can be turned into sound," says Robin Bargar, composer and NCSA visiting research programmer. "Not only have composers gained from our work, it has passed along to the scientific community."

Chaos as music

Using a unique interface, chaos becomes a musical instrument—just as musicians use the keyboard to explore the sounds of the piano or bows and strings for the violin.

"Virtual reality could learn a lot from adopting interface principles developed in musical instruments," says Bargar, who directs audio research at NCSA. "Musical instruments are some of the most sensitive real-time interactive tools made by humans."

The interface presents a digital representation of a ball that can be moved across a textured plane. Changing the peaks and valleys on the plane or moving the ball to a different area of the plane produces

different sounds. A graphic representation of the chaotic trajectory floats above the plane in the CAVE so users can see how the sound evolves.

This interface can produce sounds from almost any numerical data, which makes it valuable to scientists and composers.

Visualizing Chua's circuit

"The graphical interface provides an indispensable tool for visualizing numerous complex bifurcation phenomena, patterns, and structures associated with the topological, geometric, as well as temporal aspects of Chua's circuit," says Leon O. Chua, professor of electrical engineering and computer science, University of California, Berkeley. "It unfolds many subtle features previously hidden from view—imagine a painting drawn on the sleeves of an accordion which is hidden until the accordion is unfolded."

Chua, creator of the chaos circuit, is a leading researcher in chaos and nonlinear dynamics and editor of the *Journal of Bifurcations and Chaos*. He earned his Ph.D. in Electrical Engineering from UIUC in 1964.

An innovative interface

"By approaching the project from both ends—research-oriented and at the same time creative—we came up with an innovative interface, a manifold. The control parameter space is represented by a manifold in 3D space. From a musical point of view, this interface binds three modes of music production; in this graphic interface, composer composes, performer performs, and an audience receives orientation how sound events are unfolded," says UIUC Research Assistant in Computer Science Insook Choi, who composed a musical piece using the sounds of chaos. Her composition *anti-Odysseus, the irreversibility of time* premiered at Expo '93 in Taejeon and Seoul, Korea.

"Many scientists show research interests in terms of methods for simultaneous control of multiple parameters in a high-dimensional system," she says. "The manifold interface, developed for navigating multiple control parameters according to acoustic states related to chaotic states, provides scientists with a unique representation of the problems and potential results of multidimensional control."

Choi is a guest composer with the Audio Development Group at NCSA. She is also a professional composer of new music, concentrating on electro-acoustic and computer music.

"We are interested in using sounds of chaos to produce music and in using audio to make discoveries about chaos," says Bargar. "Historically, composers did not make the sounds they used to create music, now we can."

Bargar oversees audio research including sonification, auditory display, and the integration of audio and visual information—specifically to explore paradigms of graphic and sound computation. This includes human-computer interface development, as well as the use of sound, with traditional computer graphics and video formats.

"I am impressed and excited by all aspects of the sonification project," says Chua. "The work Robin's group is doing represents very significant pioneering research of immense commercial potential. It requires a great deal of creativity and ingenuity, as well as a very broad background, to combine high-tech hardware, programming skills, nonlinear dynamics, and music into a unique synergetic system with wonderful capabilities. It represents cutting-edge research of the first magnitude."

A new paradigm

Bargar and Choi's work uses the SGI Indigo, which is best-suited to sonification problems because of its outstanding sound computation capabilities, according to Bargar. Released in 1992, the SGI Indigo series created the potential for a new paradigm that has yet to be fully realized—even by SGI—Bargar says. "The SGI has a great graphics engine, the graphics pipeline." Through this pipeline, the Indigo does much of the graphical work for the user very quickly. There is no "equivalent audio pipeline" for Bargar.

"In addition to providing tools to science, we have to build the environment that we are going to work in," he adds. "That is both exciting and challenging."

As we went to press with this issue, members of the Audio Development Group were putting the finishing touches on a software audio pipeline of their own design. Their pipeline uses a client-server architecture that allows the SGI Indigo to perform as a real-time interactive sound synthesis engine. This system provides audio to all 43 VROOM applications at SIGGRAPH 94.

Sounds continued on page 19



The Audio Development Group: (left to right) Insook Choi, Ulrike Axen, Kelly Fitz and Robin Bargar (seated), Camille Goudeseune, NCSA/UIUC, and Sumit Das, EVL/UIUC. (Photo by Thompson-McClellan Photography)

Music out of chaos

Victor Ryckaert: What effect can your work have on music? On science?

Insook Choi: By working on the design of sound structures which reflect the behavior of systems or the structure of data, we have to consider criteria which might have not been considered otherwise; the criteria which feed our goal. 'How to design sounds for conveying information which is significant to the system behavior that we want to observe.'

This concept of sounds is neither sound effect nor 'music,' but applied to the delivery of information through the mode of qualitative observation. On music this kind of approach will make an inquiry to broaden well-comforted aesthetics and urge the community to be educated by alternative aesthetics.

On science, the community will benefit from playful observatory platforms. The graphic has been useful as a platform, with sounds it will add more to the irreducibility of our understanding of what we observe.

VR: Does it bridge any gaps between these disciplines? In what way?

IC: Was there a gap between these disciplines? The production of sounds is directly related to the physical properties of instruments and how we interplay with those instruments with an understanding of physical laws.

When we listen to Bach's Aria on G, we listen to sound waves from a resonating body traveling through air to our eardrum and activating our neurons to process the information.

This fundamental connection has been overlooked by researchers from both ends; it is the research trends which create these gaps. So I would say there are continuous paths and mutual feedback loops between these disciplines, science and music. In my work I make this relationship more explicit through digital technology by designing sound synthesis tools and simulations.

VR: What motivated you to compose music from chaos?

IC: Complex dynamical systems, such as 'chaotic systems,' have many interesting properties. From simple patterns to complex patterns, many degrees of intermittencies, characteristic transient behaviors, noise-like chaotic signals, and all these various degrees of complexity can be articulated in many levels of sounds and musical structures. It is challenging from composer's point of view not only to compose a musical piece also to build sound synthesis systems to compose with. And that sound synthesis system has to have requisite varieties to host the chaotic system and yet be perceptually differentiable. The many problems presented looked interesting enough to undertake as compositional problems.

Virtually seeing geometry by Victor Ryckaert, NCSA Student Intern



Stills from *Post-Euclidean Walkabout*, George Francis, Ulrike Axen, and Chris Hartman, NCSA/UIUC; Paul McCreary, UIUC; Joanna Mason, EVL/UIUC. © George Francis, Chris Hartman, and Glenn Chappell, NCSA 1994. (Courtesy of Francis, above; McCreary, below)

Nestled quietly among the 43 applications that are scheduled to run in the VROOM at SIGGRAPH 94 is the *Post-Euclidean Walkabout*. It is compiled from various projects that were part of a class in which students learned how to build and run their own 3D applications in NCSA's virtual environment.

"My principal goal is to teach geometry," says George Francis, UIUC professor of mathematics and long-term user of NCSA's visualization facilities. Unobtrusively labeled "Math 428—Topics in Geometry" in the UIUC timetable with the tag "Section G1 considers geometrical graphic[s]" to denote Francis's section, this one-unit graduate-level course is at the vanguard of computational science/computer graphics. Francis teaches students how to exploit the vast opportunities that virtual reality has to offer.

Francis was recently recognized for his teaching style. He won the \$1,750 Amoco Foundation Award for Innovation in Instruction.

"You start out with what you know about computer graphics and mathematics, and you work at your own pace," says Robert Schade, UIUC graduate student in mathematics who was in the class last fall. "I went in with a half-baked understanding of the [Silicon Graphics] IRIS and computer graphics. Professor Francis was very good at picking up on what I didn't know and explaining it from the ground up."

In semesters when it is offered, 10 students usually complete Francis's course. "Students continue their projects beyond the class," says Paul McCreary, UIUC teaching associate in mathematics who sat through the class each of the last three semes-

ters. Though he never officially enrolled, McCreary says he was an active participant and used what he learned to develop a thesis topic.

"I do not know if it's me or the students' natural inclination," Francis says, "my students tend to want to do things on their own. They are not great consumers of fancy software packages. Rather, they make their own codes. They learn an appreciation for doing the geometry themselves."

"I call it post-Euclidean to avoid the odd-sounding non-Euclidean geometry, which is its official name in mathematics since Gauss and Riemann," says Francis. "The similarity to post-modern is intentional, too." Francis compares the post-modern movement in the arts to what he is doing with virtual reality.

"Since Frederick Jameson's book on post-modernism, the term [post-modern] has referred to a pastiche, a quilt or patchwork, an eclectic juxtaposition of diverse stylistic elements without necessarily exhibiting any internal logic or intended structure," says Francis. "And that fits post-Euclidean best, since, in these earliest of times in the evolution of virtual reality, we explore whatever geometrical phenomena strike our fancy and fit into our limited technical repertoire."

"Walkabout is what Australian aborigines, and also native whites, sometimes do when they 'drop out' of their society for a while and wander about the waste regions of the Australian outback," he says. "The disorientation frequently experienced by CAVE visitors is alluded to here."

The goal of this project is perfecting visual and sonic environments to exhibit time-varying multidimensional geometrical shapes that interest research geometers. It is useful in applied and pure mathematics as well. ▲





Truth in science imagery

by Ingrid Kallick, NCSA Graphic Designer, USEO
Graphic by Ingrid Kallick

What makes imagery important to science? What makes scientific imagery truthful and accurate? Can scientific imagery be objectively evaluated? If so, by what criteria?

These and other questions were the focus of a symposium at the annual meeting of the American Association for the Advancement of Science (AAAS), San Francisco, in mid-February 1994. A panel of visualization specialists included Donna Cox from NCSA, computer graphics artist and UIUC professor of art and design; Karen Kaye of the NASA Science and Technology Information Program, specialist in scientific image database management; Gregory McRae of MIT, chemical engineering professor who has used visualization extensively to inform emission control policymaking; Jon Palfreman from WGBH (Boston's Public Broadcasting System outlet), executive producer for NOVA and numerous documentaries utilizing scientific graphics; and David Curtis of NCSA, creative director of scientific communications and executive producer of NCSA video programming. Curtis introduced the symposium.

Insight through images

Images have long been a part of the communication and practice of science, but the technologies that drive scientific visualization are in development. Once relegated to the static pages of textbooks and academic journals, scientific images can now be set in motion. Broadcast to homes, shown in the conference rooms of policymakers, traveling across the Internet, and being animated on computer screens, scientific images continue to expand their role as visual interlocutor between research scientists, the media, and policymakers.

"This panel seeks to address a specific need, namely that in an image-hungry society like ours, a keener awareness of the elements of 'truthfulness' or 'validity' of scientific imagery and visualization is desirable for a greater understanding of science—and particularly its impact on society," said Curtis in his introduction.

Animation and video media have transformed scientific images into powerful storytellers. Yet how reliable are their stories? Conceptual illustration and data-driven visualizations are often used interchangeably. While data-driven images are usually considered to be more valid, the relative validity of one form over the other is not always clear.

Illustrations are subjective pictures of scientific concepts, yet the supposed objectivity of data-driven visualizations from numerical simulations may not be so different. In visualizations there is no one-to-one correspondence between data and representation, and the process of numerical simulation introduces subjective elements. In a recent article in *Science* [1], the difficulty of evaluating numerical simulations was discussed. Similar concerns have prompted the DoE to begin work on standards for evaluating numerical simulations of ground-water pollution. [2]

NOTE: This AAAS panel was organized by Ingrid Kallick and David Curtis of NCSA and Bonnie Carroll, Secretariat-Director of CENDI (Commerce, Energy, NASA, National Library of Medicine and Defense Information management group). For further discussion of this topic, see Ingrid Kallick's article, "Science Icons: The Visualization of Scientific Truths," in a forthcoming issue of *Leonardo* (volume 27, number 4, 1994).

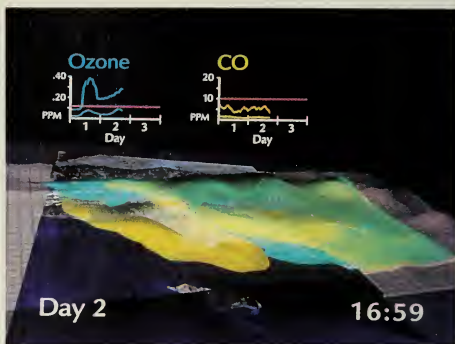
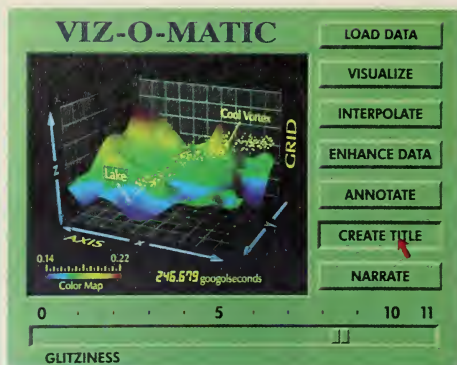
The debate about standards for visual representation persists along with questions about numerical simulations. This was illustrated by an animation from the Cornell Theory Center by Animator/Producer Wayne Lytle called *The Dangers of Glitziness and Other Visualization Faux Pas*, using fictitious software named "Vizo-Matic." [3] The video, shown in the Electronic Theater at SIGGRAPH 93, documents the enhancement and subsequent "glitz buffer overload" of a sparsely data-driven visualization trying to parade as a data-driven, thoughtfully rendered presentation. (See Figure 1, page 16.) The video was a humorous response to discussions at an April 1992 meeting of the MetaCenter visualization community at SDSC.

Insight gained

Though some might question any use of "glitzy" graphics, McRae argued for using persuasive and sophisticated—if not exactly glitzy—visualizations. "Imagery and images are extremely important in the policy process. . . . In order to be able to interpret whether or not an image may be telling you the truth requires a level of understanding and education."

McRae says that to inform a decision-making body of basic scientific concepts, it is imperative to have a presentable visualization. With examples of his work on monitoring air pollution in Los Angeles and Mexico City, he sought to demonstrate that a carefully crafted and readable visualization will do just that. (See Figure 2, page 16.) For McRae's purposes, the risk of possible misinterpretation of visualizations was secondary to the benefits of the audience understand-

Truth continued on page 16



Truth continued from page 15

ing the science. As McRae reminded the AAAS audience, "The purpose of computing is insight, not numbers." [4]

Insight in question

More recently, concern has grown in the visualization community and the science media over the use of scientific imagery, its interpretation, and the relation of the data to its interpretation. Computer manipulation of images, in the general sense, has been a subject of interest in the popular press. Appearance is important to the interpretation of a scientific image, but not solely. Context, narration, sound, authority and viewpoint of presentation, editing, and reliability of and amount of underlying data contribute to the meaning of a scientific image; all can give very different interpretations to the same design.

Palfreman emphasized the metaphorical qualities of imagery in his presentation, stating, "Like literary metaphors, the visual metaphor aids communication by suggesting how a new unfamiliar thing—for example, the life cycle of the HIV virus—can be thought of in more familiar terms." Science is presented as a story or a metaphor. In light of this, scientific imagery must be evaluated as information, as well as design, demanding a broader view of both.

When they are removed from the scientific research, poorly labeled, or shown in a sequential video without context, scientific images tell little about the procedures that generated them. Intentionally or unintentionally, the use and reuse of such images

Figure 1, left (Courtesy of Wayne Lytle, CTC); Figure 2, right (Courtesy of NCSA).

may mislead viewers. Texts in scientific journals are formally peer reviewed, but scientific imagery is not.

Cox emphasized that peer review may be the necessary step in improving the credibility of scientific visualization as a vehicle for insight into data. "There are currently real problems with the... untestability of visualization techniques... We do not have peer review of the algorithms, data sampling techniques, standards for spatial/symbolic mapping, or the methods for representing the data. This condition places scientific visualization in a precarious position."

Cox said that usually the intended audience and message determine the form of a visualization. It is imperative to have this information when evaluating a visualization or other scientific imagery, and it should be passed on when images are placed in a new context.

New contexts, new media

The computational environment of visualization is currently experiencing an explosion of online capabilities.

Kaye presented solutions for documenting, accessing, and scrutinizing scientific imagery online, including a NASA Home Page and image database using NCSA Mosaic with (currently restricted) access to the underlying visualizations.

NCSA's numerical relativity exhibit and digital library (see URLs below) are also being expanded to include detailed information about NCSA scientific imagery.

Another example given was Al Globus's "Annotated Scientific Visualization URL Bibliography," which provides useful information about what visualization resources exist online (see URL below). Globus is a research assistant at NASA Ames Research Center.

Truth continued on page 27

NCSA numerical relativity exhibit: <http://jean-luc.ncsa.uiuc.edu/>

NCSA digital library:
<http://www.ncsa.uiuc.edu/SCMS/DigLib/text/overview.html>

A. Globus's "Annotated Scientific Visualization URL Bibliography":
<http://www.nas.nasa.gov/RNR/Visualization/annotatedURLs.html>

ZEUS code simulates comet crashing into Jupiter

by Victor Ryckaert, NCSA Student Intern

As shattered remnants of a comet orbiting Jupiter hurtle towards the giant planet, researchers are trying to understand—through computer simulation—how the comet fragments will affect Jupiter's atmosphere. In a MetaCenter collaboration, Mordecai-Mark Mac Low is using ZEUS software [see *access*, Spring 1994] created by NCSA's Laboratory for Computational Astrophysics (LCA) running on the Pittsburgh Supercomputing Center's CRAY C-90 system.

Fragments of the comet Shoemaker-Levy 9 are going to dive into the gaseous planet Jupiter between July 16 and 22 and vaporize just behind the limb of the planet out of view from Earth, scientists say. Astronomers hope to see the explosions reflected off Jovian moons or perhaps through cameras of the crippled Galileo Orbiter. About 20 minutes after each collision, the impact site will rotate into view giving researchers an opportunity to view the aftermath from Earth or from orbiting telescopes, such as the Hubble.

"It is a real disappointment. Something like this only happens every couple of hundred years," says Mac Low, an astronomy research associate at both the UIUC and the University

of Chicago. "It is the biggest solar system event of our lifetimes, and it is happening on the wrong side of the largest planet."

Mac Low's experience using ZEUS codes gave him a headstart on the comet simulation. "Mordecai is our primordial ZEUS user," says LCA Director Mike Norman. "He has been riding the ZEUS technology curve since 1987."

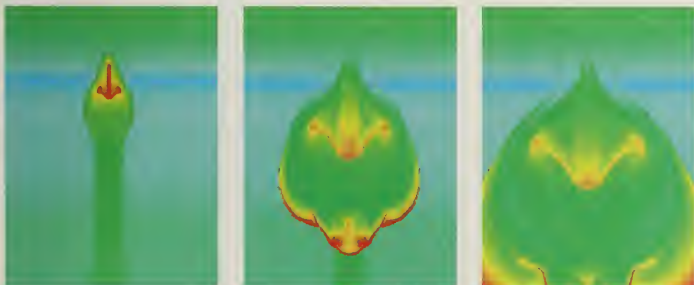
Mac Low was—and still is—using ZEUS codes to examine superbubbles [see *access*, May–June 1987], which form when many stars become supernovas in a small region. He was able to quickly retool this and another related project in order to study the comet crash. Mac Low was also using ZEUS to simulate a cloud of interstellar gas getting hit by a supernova shock wave. By treating the comet as a gas—because of its speed and density compared to the Jovian atmosphere—and using his superbubble models to study the fireball resulting from the impact, Mac Low was able to get preliminary results quickly.

Mac Low's comet research has stirred some debate because it disagrees with the results of other computations of the altitude of the comet explosion. Some of his competitors found that fragments would simply

be absorbed by Jupiter's gaseous atmosphere. Mac Low's simulation was computed using 200 gridpoints across the comet, while the other simulations used only eight gridpoints across the comet. According to Mac Low, the low resolutions do not show the comet's explosion and fragmentation.

If the calculations are supported by observations, Mac Low and his collaborator, Research Scientist Kevin Zahnle of NASA Ames Research Center, will apply their theory to the Earth. "The big question is: How big a rock will the Earth's atmosphere protect us from?" Mac Low says. If their model is right about Jupiter, it could be adapted to make predictions about asteroids that may one day head for Earth. ▲

Simulation of the fireball resulting from a comet, 1 kilometer in diameter and made of solid ice, hitting Jupiter. Times shown are 30, 50, and 90 seconds after impact. Temperatures are on a log scale with blue a few hundred degrees Kelvin (K); red, close to 10,000 K—hotter than the surface of the sun. Darkest blue stripe represents the top of the clouds. (Courtesy of Mac Low) Mordecai-Mark Mac Low, right. (Photo by Victor Ryckaert, NCSA)



FMC RECEIVES NCSA GRAND CHALLENGE AWARD

BY FMC CORPORATION



FMC researchers Mike Skreiner, left, and Ernie Plummer, right, display their Grand Challenge Awards presented by NCSA Director Larry Smarr, center, at the Sixth Annual Executive Meeting of NCSA's Industrial Partners (above). Partner executives and NCSA staff convened at the Beckman Institute to discuss advancements in HPCC technologies and their relationship to business strategies (below). (Photos by Wilmer Zehr Photography)

FM C Corporation, headquartered in Chicago, received top corporate honors from NCSA at the center's Sixth Annual Executive Meeting of NCSA's Industrial Partners in April 1994.

FMC was recognized for its use of modeling and simulation employing high-performance computing technology to enhance research applications in the areas of controlling insect pests and weeds, as well as optimizing machinery, vehicles, and chemical processing plants.

"For FMC, earning NCSA's third Industrial Grand Challenge Award began with the creation of prototypes to model new products and processes," says John Stevenson, NCSA's corporate officer and head of the Industrial Partnership Program. "Our partnership helped provide FMC with the appropriate technology and access to high-performance computing."

FMC succeeded in performing dozens of modeling and simulation projects to improve current products and contribute to the development of new products. The technology developed by FMC scientists and engineers is being used at FMC's Corporate Technology Center in Santa Clara, CA, and at a range of FMC businesses—including agricultural and industrial chemicals, energy equipment, food machinery, and airline and defense equipment. HPC capabilities are increasing the efficiency of processes and contributing to cost savings.

FMC also produced unique 3D models of an enzyme and a receptor protein, both used to design new compounds for pest control. This provides FMC research and discovery scientists with the ability to visualize and test their ideas in simulation before committing FMC's resources to synthesis, resulting in significant savings.

The award recognizes the efforts of Mike Skreiner (FMC's Corporate Technology Center in Santa Clara, CA), Ernie Plummer (FMC's Agricultural Chemical Group at the company's Research and Development Center in Princeton, NJ), and their teams of technologists.

"We made the decision almost six years ago to invest in high-performance computing, modeling, and simulation," Skreiner states. "It was at that time that we began working with NCSA. Our task was to pioneer the access, exploration, and transfer technology to provide significant business benefits to FMC's worldwide operations. That led to some real opportunities and applications, such as the research and discovery work of Dr. Plummer and his team in Princeton."

"We focused our work on the development of three-dimensional models of enzymes and receptors—targets for the control of insect pests and weeds," Plummer explains. "We applied high-performance computing to enhance our discovery process. We isolated the building blocks that dictate insect growth—enzymes and receptors—then built three-dimensional models of them. We then were able to test models of new compounds against the target sites to estimate effectiveness.

"Being able to visualize this interaction with the target site allows our scientists to use their imaginations, and increases the probability of finding new compounds," Plummer says. "We can actually visualize how a compound interacts with a target site and what changes we can make in order to increase its activity. The electronic images are dynamic models that move like the real world moves and give us a much more accurate view of what we are seeing."

"One of the other reasons for establishing our relationship with NCSA and UIUC was to improve the efficiency of FMC's operations," Skreiner points out. "That's clearly happened, too. By developing a better understanding of high-performance computing, we were able not only to plan and justify new acquisitions, but also to determine when to dispose of obsolete computing resources. Since 1988 we have reduced our cost of a unit of computing 1,900 times."

The partnership between FMC and NCSA could result in scientific innovations that bring competitive advantages to U.S. businesses on a global scale. For FMC, the partnership is an important step in expanding its leadership position in the global marketplace. FMC joins 11 other major corporations as part of an industry-university-government partnership to help American industry advance in the use of HPCC. ▲

New NCSA Mosaic licensees

Updated listing of NCSA Mosaic new licensees as of early May 1994 that continue from that in Spring 1994 access:

Electric Power Research Institute (EPRI)^{*}
Palo Alto, CA
Spyglass Inc.^{*}
Savoy, IL
Ubique Ltd.^{*}
Israel

^{*} NCSA Mosaic platforms licensed: X Windows, Macintosh, and Microsoft Window System

NCSA Mosaic is free for academic, research, and internal business purposes (see access, Spring 1994). Nonexclusive licenses are necessary for commercial use and redistribution. Licenses can be written for one version or all three versions of NCSA Mosaic. Companies have the option of using updates as they become available.

OCTOBER SYMPOSIUM: COMPUTATIONAL MOLECULAR DYNAMICS

The University of Minnesota Supercomputer Institute is hosting an international symposium on Computational Molecular Dynamics, October 24–26, 1994, at the Hubert H. Humphrey Center on the University of Minnesota campus, Minneapolis. The symposium will cover all aspects of the dynamics of molecular systems and the use of molecular dynamics simulations—quantum and classical, few-body and many-body, physics and chemistry.

In addition to the invited talks by internationally renowned speakers, there will also be poster papers. The organizing committee anticipates that a fruitful exchange of information will occur—given the broad group of computational chemists and physicists expected to attend.

Contributed poster papers are invited and strongly encouraged. Persons who wish to present a poster should send a one-page abstract by July 25, 1994. Late posters will be accepted on a space-available basis.

The symposium is sponsored by the University of Minnesota Supercomputer Institute; the Computers in Chemistry Division, American Chemical Society; the Division of Computational Chemistry, American Physical Society; and the Physical Chemistry Division, American Chemical Society. Symposium organizers are: Jan Almlöf (U. of Minnesota), Evelyn Goldfield (CTC), M. Katharine Holloway (Merck Research Labs.), William Jorgensen (Yale U.), Peter Rossky (U. of Texas at Austin), George Schatz (Northwestern U.), and Donald Truhlar (U. of Minnesota).

Registration for the symposium is \$150 for submissions prior to September 30; \$175 for those after September 30. A 10% discount will be given to members of the cosponsoring divisions of the American Chemical Society and the American Physical Society.

For more information, contact the Symposium Administrator Michael J. Olesen, Supercomputer Institute, U. of Minnesota, 1200 Washington Ave. South, Minneapolis, MN 55415; phone: (612) 624-1356; FAX: (612) 624-8861; email: olesen@msi.umn.edu (Internet). ▲

Sounds continued from page 13

In addition to Bargar and Choi, Ulrike Axen, Kelly Fitz, Camille Goudeseune (NCSA/UIUC), and Sumit Das (EVL) form the Audio Development Group.

"We know sound enhances our lives; the spoken word tends to be more convincing than the written," says Bargar. "Numerical data converted directly into sound becomes qualitative. We are not improvising or making up the data. We postulate that there are ways of interpreting data that are still unknown." ▲



What's

A fifth-grade student from Champaign, IL studies a real-time surface analysis map and the latest radar summaries to make the same prediction that the weather forecaster would make on the evening news that same night. Several inches of snow, accompanied by blustery winds, would hit much of Illinois the next day. Is this the work of an exceptionally precocious Willard Scott? Not necessarily.

Students in John Blair's fifth grade class at Champaign's Washington School are using NCSA Mosaic, a global hypermedia-based information discovery, retrieval, and collaboration system built atop the World Wide Web (WWW) technology [see *access*, Fall 1993; Spring, 1994], to access up-to-date weather data on the university's Weather Machine, a service provided by the UIUC Department of Atmospheric Sciences. With the help of Blair and Don Crockett, a graduate research assistant in NCSA's Education Group, the students forecasted the February 25 winter storm that closed highways over a large portion of the state.

NCSA Mosaic bridges the gap Blair's class is taking part in what could be called, with little exaggeration, a revolution in science education—an approach to learning that gives children the same tools and data available to scientists. In short, an approach that allows children to be scientists. This is exactly what NCSA's Education Group hopes to

accomplish: to bridge the gap between classroom science and the kinds of scientific research done by professional mathematicians and scientists [see *access*, Spring 1994].

"Building a good bridge not only requires a basic roadbed, but—if it is to handle large amounts of traffic—a support system in the form of cables and trestles as well," says Bob Panoff, member of the Education Group and SuperQuest '94 instructor. "In our effort to bridge the gap between education and science, we have built a support system in the education courses and workshops we offer to teachers. These have undergone a tremendous increase in popularity since last summer."

According to Panoff, major factors for increased interest in the courses and workshops are the installation of ISDN lines (Integrated Services Digital Network lines, high-speed network connections) in some local schools [see *access*, Fall 1993] and the statewide and national interest in networking due to the NII.

NCSA Mosaic is one of the newest tools helping to bridge the gap [see *access*, Fall 1993; Spring 1994].

While students could theoretically access any of the weather data with a network connection through a Gopher server [see *access*, October–December, 1992], NCSA Mosaic, which is essentially hypercard on a global scale, allows the teacher to design a document appropriate for the classroom. With NCSA Mosaic, the teacher can select data or images available on the

Internet s/he wants the students to access, and add context around that information. For example, a student may click on an icon to view a satellite image from the Weather Machine and another to view data on pressure systems. Another click brings up text written by the teacher explaining the relevance of pressure systems or the methods used to generate satellite images; click again, and the student views an archived video depicting a winter storm.

"By focusing on current data, the teacher can highlight the relevance of different concepts and why they are important in forecasting," says Crockett. The possibilities for making science come alive are great, according to Crockett: "If a current satellite image shows a front coming through your area and you look out the window and see a clearly defined boundary between clear blue sky and fast moving clouds, your understanding of frontal systems becomes much more relevant."

Collaborative visualization in the classroom

The atmospheric sciences—which can teach students a great deal about physics, chemistry, geography, mathematics, geology, and environmental issues, as well as weather and meteorology—are at the heart of another science education testbed project called CoVis (Learning through Collaborative Visualization). In this project, members of NCSA's Education Group and the UIUC Department

blowin' in the wind?

A revolution in education *by Sara Latta, Science Writer; illustration by John Havlik*

of Atmospheric Sciences are collaborating with faculty and students at Northwestern University's (NWU) School of Education and Social Policy, teachers at two Illinois high schools, and the Exploratorium Museum in San Francisco. (See sidebar, page 22.)

Students participating in the CoVis Project study atmospheric sciences through project-based activities. They may investigate the reasons for the exceptionally cool summer of 1993, for example, or Lake Michigan's effect on Chicago-area storms.

The CoVis Project provides students with a "collaboratory" workbench: desktop video teleconferencing; shared software environments for remote, real-time collaboration with other students, scientific mentors, and other experts; access to resources on the Internet; instructional modules; and scientific visualization software.

"Among our primary research goals in the CoVis Project," says Barry Fishman, graduate student in NWU's School of Education and Social Policy, "is to determine the level of technology required to support cross-school and cross-community collaboration, and to use that data to help shape educational and telecommunications policy at the state and federal level."

Mythili Sridhar, graduate research assistant in NCSA's Education Group, and Steve Hall, graduate student in UIUC's Department of Atmospheric Sciences, developed hypercard multimedia instruction modules on topics such as pressure, forces and winds,



and weather maps for CoVis. The modules incorporate colorful diagrams, video clips, text, and audio narration in what amounts to an interactive, online textbook. For example, one video demonstrates the Coriolis force by showing the curved path a ball takes when rolled by children on a whirling merry-go-round. (The *Coriolis force*, introduced by French Physicist Gaspard de Coriolis in 1835, is a fictional force used to simplify calculations about rotating systems: the movement of air, water, and projectiles over the Earth's rotating surface.)

"Students are interested in anything they can learn on the computer," says John Blair, teacher at Champaign's Washington School. Tu Nguyen, Crystal Hardyman, and Heather Davis (left to right) agree.

(Photo by Thompson-McClellan Photography)

Blowin' continued on page 22



CoVis Project

Sponsors
 National Science Foundation
 Applications of Advanced Technology
 Informal Science Education

Lead institution
 Northwestern University

Institutional partners
 UIUC Department of Atmospheric Sciences
 The Exploratorium Museum (San Francisco)
 Technical Education Research Center, University of Michigan

Industry partners
 Aldus Software
 Ameritech
 Apple Computer Inc.
 Bellcore
 Farallon Computing
 Science Kit and Boreal Labs
 Sony
 Sun Microsystems

Participating Illinois high schools (Phase 1)
 Evanston Township High School, Evanston
 New Trier High School, Winnetka

Blowin' continued from page 21

Using NCSA Mosaic

The release of NCSA Mosaic has given Sridhar and Hall an even better tool for constructing the modules, and they will eventually convert existing hypercard modules for display using NCSA Mosaic. In fact, Mohan Ramamurthy, UIUC professor of atmospheric sciences and head of the UIUC CoVis Group, says, "[NCSA Mosaic] solved a series of problems when it came out. We were doing interactive multimedia, but not across the network. We wanted to set up some sort of digital library that provides access to real and retrospective databases, to educational modules, and so on. In one shot, Mosaic allows us to do that."

NCSA Mosaic also allows users to integrate all of the multimedia features used in the hypercard modules, without taking up the space. "With hypercard, we had to send the entire package," said Hall. "In some cases, that would be 50 megabytes. Mosaic allows the teacher to pick and choose the parts of the module that are needed and get them over the network."

NCSA Mosaic enables students to link to different Gopher servers, FTP, and WWW sites, so that moving from

UIUC's Weather Machine Server for up-to-the-minute weather data and then to the Exploratorium Server for meteorological demonstrations involves clicking on highlighted words.

A revolution

These projects represent a major departure—a revolutionary approach—from the standard textbook-based, fact-memorizing concept of science education. They encourage students to learn about science by being scientists, using the same tools, the same data, the same network connections as university scientists.

Blair's fifth grade students like the change. "Once we had the system [NCSA Mosaic] working well, they were very enthused and wanted to learn as much as possible," he says. "They are interested in anything they can learn on the computer."

"School is unique in the amount of isolation it forces on the learning process," says Fishman. "In many [schools], even collaborating with the student sitting next to you is considered 'cheating.' We are trying to foster an atmosphere where students, teachers, and scientists can work together as peers—regardless of their physical location. For that, the technology is absolutely essential." ▲

CoVis Project's WWW Server: <http://www.covis.nwu.edu>

New consulting hours

NCSA's National Consulting Office announced new hours effective the beginning of June 1994. New hours are from 8:30 a.m. to 5:00 p.m. (CT).

The extended hours, advertised to users earlier this year [see *access*, Spring 1994], did not generate the expected level of calls and electronic mail inquiries according to John Towns, team leader of the consulting staff. Send any comments or questions to the Consulting Office (see *nlsa contacts*, page 2). ▲

Best of the Web '94

While in production, the Best of the Web '94 Awards nominees were presented at the First International World Wide Web Conference, Geneva, Switzerland.

NCSA won for Best Overall Site. According to Brandon Plewe, Best of the Web '94 Coordinator from SUNY/Bufalo, the center will be able to display a "virtual award" and use the BoWeb'94 logo on its NCSA Mosaic Home Page.

Awards were given in 14 categories. A permanent awards exhibit is on the World Wide Web (WWW) via NCSA Mosaic (see the URL below).

For further information, contact Brandon Plewe at plewe@acsu.buffalo.edu (Internet). ▲

The Best of the Web '94: <http://wings.buffalo.edu/contest/>

METACENTER ONLINE INFORMATION

BY GINNY HUDAK-DAVID, NCSA PUBLICATIONS EDITOR, PUBLICATIONS GROUP

Do you want to know about JNNIE, a joint NSF-NASA project to evaluate scalable parallel computing under real-life scientific conditions? How about the current training schedule for one of the centers participating in the National MetaCenter? Do you just want to know what the MetaCenter is?

That information and more is available in the National MetaCenter document accessible by using NCSA Mosaic [see *access*, Fall 1993], the software program from NCSA's Software Development Group that is taking the Internet by storm. NCSA Mosaic retrieves information from servers (World Wide Web, Gopher, or anonymous FTP) then formats and displays it on your workstation.

Your choices

Information available on the MetaCenter Home Page falls into one of four categories:

- **General information**—How to obtain an allocation, contacts list, publications, and links to the World Wide Web servers at the participating institutions
- **Research at the MetaCenter**—Science highlights online, technical reports and bibliographies, and research datasets
- **Education programs in HPC**—Programs/workshops/training/user support information, K-12 and college-level programs, and educational contacts
- **Collaborative projects**—JNNIE project, science highlights online, and conference exhibits

If you do not have NCSA Mosaic

You can obtain NCSA Mosaic from NCSA's anonymous FTP server (<ftp.ncsa.uiuc.edu>). See the inside back cover of *access* for instructions. NCSA Mosaic is available for the X Window System, Macintosh, and Microsoft Windows. The default start-up document (called a *home page*) is the NCSA Mosaic Home Page.

Accessing MetaCenter information

Once you are up and running, select Open URL . . . from the File menu. In the field provided, enter the URL shown in the box below.

The online information world is available with the click of a mouse. ▲

MetaCenter Home Page: <http://www.ncsa.uiuc.edu/General/MetaCenter/MetaCenterHome.html>



NCSA MOSAIC INTERNATIONAL CONFERENCE

NCSA together with NSF, the Open Software Foundation Research Institute, and UIUC are cosponsoring the Mosaic and the Web international conference '94 at the Ramada-Congress Hotel, 520 South Michigan Avenue, Chicago, on October 17-20, 1994.

Participants will include up to 1,000 individuals from the public and private sectors—academic, business, and government—who are being affected by the exponential growth of the information superhighway. The program includes the "latest and greatest" innovations for navigation along the information superhighway.

Sessions on information discovery, HTML (hypertext markup language),

information security, server administration, and much more will be presented. There also will be discussions with the NCSA Mosaic development team.

The dramatic technological achievement of NCSA Mosaic and the World Wide Web are affecting the lives of people globally. The information superhighway also presents a new paradigm for education and provides an opportunity for the federal government to energize the nation in a positive way. The vision is that every individual will become both viewer and author with interactive

participation and access to knowledge. This new method of communication may create a community around the world that will not know boundaries of wealth or poverty, age, sex, nationality, or race.

An online call for papers, panels, and presentations was made in May. To obtain information regarding the Call for Papers, send email to bkucera@ncsa.uiuc.edu

To request **registration information**, send email to well@osf.org or call 1-626-621-7343. For **current information**, keep an eye on the URL below. ▲

NCSA Mosaic conference: <http://www.ncsa.uiuc.edu/SDG/IT94/IT94info.html>

LETTER TO NCSA USERS

April 1994

To: NCSA Users

From: Larry Smarr, Director of NCSA

NCSA's strategy for meeting the computational requirements of its users is evolving in response to both advances in technology and changes in federal funding policy. NCSA will be phasing out some platforms and adding new ones this calendar year in an effort to offer our users an increased level of parallelism on both distributed and shared memory architectures that employ microprocessor-based technology. These new scalable architectures not only will be upgrading much faster than traditional vector machines, but will also be more software compatible with widely used desktop workstations manufactured by vendors such as Silicon Graphics Inc. (SGI) and Hewlett-Packard (HP).

In particular, the Connection Machine Model 2 (CM-2) will be retired from production on May 2, 1994, and the CRAY Y-MP4/464 system will be turned off on September 30, 1994, at the expiration of its lease period. These machines have been the backbones of our computational offerings over the past four years—the CRAY Y-MP providing a stable platform for traditional vector supercomputing applications and the CM-2 serving as our initial massively parallel architecture machine. Our CM-2 users' successful applications (as well as the amount of time they used) led to the acquisition and production use of the distributed memory 512-node Connection Machine Model 5 (CM-5), which NCSA will retain and plans to upgrade within a year. NCSA has no plans at this time to replace the CRAY Y-MP with a vector multiprocessor architecture.

Instead NCSA will move to scalable, shared memory platforms constructed from microprocessors. These platforms have a rich software environment familiar to us on our local workstations. NCSA has chosen to deploy the new scalable machines from SGI and Convex Computer Corporation. These high-performance platforms are binary compatible with the hundreds of thousands of workstations from SGI and Hewlett-Packard respectively.

An SGI 32-processor Challenge has been in place since May, replacing the 8-processor Challenge installed in February. The 32-processor Challenge machine has twice the peak performance and quadruple the memory of the current CRAY Y-MP. It will be upgraded to a 16-processor TFP Power Challenge in July, offering even higher overall performance. SGI currently offers more parallel third party applications than any other vendor.

The CONVEX C3880 will remain at NCSA at least through its lease period that ends September 30, 1994. A CONVEX Exemplar machine arrived April 22, 1994, and consists of a single hypernode of 8 processors and 512 Mbytes of shared memory. This system has a peak speed of 1.6 Gflops, compared to 1.0 Gflops for the CONVEX C3880 and 1.3 Gflops for the CRAY Y-MP. Pending funding approval, plans call for the upgrade of this system to a 64-processor, 8-Gbyte system by the end of calendar 1994 with another doubling scheduled in 1995. The 64-processor machine will provide a peak speed increase of a factor of ten times over the current CRAY Y-MP system. As the Exemplar becomes fully functional, it will replace the C3880.

This letter serves as notification of these pending system changes. Project Principal Investigators will receive hard copy of this letter as well as an extended analysis of the upgrade strategy and suggested scenarios for migrating codes to the new platforms. NCSA is dedicated to making the transition to these new systems as smooth as possible for our users.

Questions and comments on these plans are encouraged, and may be sent via email to future@ncsa.uiuc.edu. We are excited by the ability to offer these new systems to the national user community and trust that they will greatly enhance your performance and productivity.

NOTE: The extended analysis is also available on NCSA's World Wide Web server at the following URL: <http://www.ncsa.uiuc.edu/General/Strategy/StrategyHome.html>

VISUALIZING NATURE

BY KENNETH CHANG, NCSA RESEARCH PROGRAMMER, PUBLICATIONS GROUP

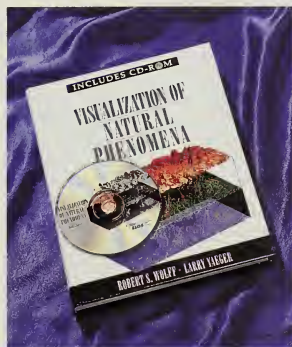
Multimedia, though having made it to the cover of *Time*, is still in its formative years—a revolution still in search of purpose. Pretty pictures, impressive soundtracks—but people are only now beginning to mold it into something more than MTV for the computer.

Scientific computing, too, has entered the age of the CD-ROM with its share of achievements and disappointments. In the impressive category is *Visualization of Natural Phenomena* by Robert S. Wolff and Larry Yaeger of Apple Computer Inc. It is not even multimedia; it is a clearly written, beautifully illustrated 374-page encyclopedia of scientific visualization. Mixing the field's history, explanations of visualization techniques, and wonderful examples, the book is enjoyable for anyone—from neophyte to expert—to page through.

Caution: Technical lingo

Note though, sections of the book are quite technical in nature, and the casual reader is likely to glaze over at sentences like, "However, instead of using a (u, v) parametric mapping based purely on the object's geometry, the mapping is based on the direction of a reflection vector computed by reflecting the vector from the eye to the point on the object's surface about the surface normal at that point." The writing is still clear, if you care about such matters; otherwise, just skip to the more interesting sections, like Chapter 7, which discusses the cross-pollination between scientific visualization and Hollywood special effects.

Bundled with the book is a CD-ROM. The CD succeeds both as a supplement and by itself. Icons in the margins of the book tie the two together, referring the reader to a specific clip that clarifies a point the authors are making. For example, one section of the book discusses the "spokes" found in the rings of Saturn. From the image in the book, the spokes are not immediately obvious—they rather look like unintentional smudges. When the corresponding movie is viewed, however, the structures immediately become apparent.



(Photo by Thompson-McClellan Photography)

Like sitting in on SIGGRAPH

By itself, the CD-ROM is still a fascinating experience and avoids the mistake of many such projects of simply parroting what has already been said in the book. With animations ranging from Egyptian mummies to Sony commercials, it is rather like sitting in on the animation festival at SIGGRAPH's annual computer graphics conference where thousands gather to goggle at the latest gadgets and wow at the computer animations. The disadvantage is that the 180 x 240 pixel window is no substitute for the multistory screens at SIGGRAPH, but the advantages are twofold. Next to each animation is a short, clear explanation of what the animation shows and the techniques used—a context for the pretty pictures. The other advantage, for people in the visualization field at least, is that the viewer can immediately refer back to the book to read up on the details of a given technique.

The particulars

Two useful appendixes describe the production environment—including hardware, software, and data management—created by the authors (Appendix A) and provide a lengthy glossary of terms and a reference list (Appendix B).

NCSA staff members who contributed to the book include Director Larry Smarr (Foreword; images and information), Research Scientist Mike Norman (technical review), and SDG Management Analyst Susan Goode (data and software). ▲

Minimum system requirements: Apple Macintosh II or later; System 7.01 or 7.1; 8 Mbyte RAM; 13-inch RGB monitor (8-bit color minimum); 5 Mbyte free hard disk space; CD-ROM drive; QuickTime 1.5 or later needed to play movies on CD-ROM.

Published by TELOS, The Electronic Library of Science, an imprint of Springer-Verlag (New York: 1993); ISBN: 0-387-97809-7.



Virtual continued from page 8

Such teams are "necessary to integrate virtual environments into the computational science discovery process and to discover—literally—usable paradigms for virtual environments in the NII."

CyberKids

Conference events are not limited to working scientists and engineers, as Brown points out.

"A portion of VROOM and its development will be devoted to children. Experiences will be developed by children and created for children to showcase the role of high-end visualization in K-12 mathematics and science education," she says. The CyberKids program will closely coordinate with the SIGGRAPH 94 SIGKids event.

Coco Conn, SIGKids chair in 1992 and 1993, and Zane Vella of the Four Oaks Foundation will be implementing CitySpace. "The project will use the city building as a metaphor for collaborative construction of content-specific areas," Brown says.

Prior to the conference, children were invited to develop VR experiences for four city buildings: "The Astronomer's Workshop," "The Fractal Theater," "The Music Shop," and "The Human Body Shop." They may also construct their own locations/buildings. A team of children and mentors will incorporate submissions into CitySpace at several workshops.

Industrial outreach

Virtual environments are also becoming an integral step in the design process of NCSA Industrial Partners Caterpillar Inc. and FMC Corp.

For several years, Caterpillar has been using VR at NCSA to design backhoe loaders and wheel loaders [see *access*, Fall 1993]. Their work has used a combination of a helmet and specially built platforms as the interface, with the goal of increasing operator visibility. Plans call for exploring the CAVE environment as well.

"The CAVE allows the operator of a vehicle simulation to have a large field of view and still maintain fairly good graphics resolution," says Richard Ingram, academic liaison at Caterpillar. The company will display some of their efforts at VROOM.

FMC has explored several VR interfaces for analysis in design work (see page 18) and will be working on a major project in the CAVE this year, says John Luranc, director of Manufacturing and Engineering Computing at FMC.

Challenges to overcome

A more long-term development will incorporate HDTV. "The CAVE is functionally twice the resolution horizontally and equal to HDTV resolution vertically for a four-screen CAVE," DeFanti says. "The workstation standard is not the same as the broadcast TV standard, though. We want to be compatible with the broadcast standard, in part so that we can make videotapes, which is not possible to do directly off a workstation now."

VEG will be working with Thomas Huang's Image Formation and Processing Group at UIUC, which received a million-dollar NSF grant in 1992 to research HDTV.

Topological Surface Deformation—Alan Verlo, EVL/UIC, and Lou Kauffman, Dept. of Mathematics, Statistics, and Computer Science, UIC, left. *A Walk through Chesapeake Bay*—Eileen Hofmann, Larry Atkinson, John Klinck, Arnoldo Valle-Levinson, and Glen Wheelless, Center for Coastal Physical Oceanography, Old Dominion U., right. (Courtesy EVL/UIC)

One area of application is robotics. "You can put a robot in a hostile environment, for example, and see what it is recording through the CAVE's 'eyes,'" DeFanti explains. "This would be integrated with broadcast TV and would be good for deep sea or planetary exploration."

More fundamentally, "VR is heading towards having to invent usable methodology," DeFanti says. "It is precisely where scientific visualization was in 1986—a few smart practitioners, but only the beginnings of clear paradigms of utility."

He describes current VR as just becoming usable for scientific explorations. "I believe we need teraflop computers and 100 Gbps [gigabits per second] networks to get VR to the quality of still images and high-end animations," DeFanti says. "How we get where we want—record it, get back to it, share it, teach it—are all the big challenges." ▲

Wanted: Technology stories

Kathleen Wiegner, who is starting a weekly column for the *Los Angeles Times* called "In Development," is looking for interesting technological developments in a wide number of fields. She wants suggestions for interesting articles.

Her email address is 508.5600@mcimail.com; phone is (505) 829-3109; FAX (505) 829-3110; mail address, P.O. Box 599, Jemez Springs, NM 87025.

FLASH! World's largest computer simulation of the universe on CM-5

by Neal Singer, UIUC News Bureau

The newest and largest super-computer simulation of the universe agrees so well with astronomical observations that it may point astronomers toward discoveries in unexplored sectors of the universe, says NCSA Research Scientist Mike Norman, who led the effort. The simulation, run on NCSA's CM-5, visualizes the universe as it would be seen by x-rays, said Norman, UIUC astronomy professor and team leader of NCSA's Astrophysics Group. (A video of the simulation is available from Norman.)

"This is the largest cosmological simulation of the view that x-rays would give of the universe," Norman said. "Our simulation is the first that is sufficiently comprehensive to make theoretical predictions that can be compared with observations."

The model, funded by NASA and NSF, was announced June 1 at a meeting of the American Astronomi-

cal Society in Minneapolis, MN. Based on algorithms by UIUC graduate student Greg Bryan, the simulation models the effect on cosmic gases of a theory that the universe contains cold and hot dark matter. The simulation closely matches recent x-ray observations of galaxies by ROSAT, NASA-European Space Agency satellite.

Consuming 30 wallclock hours on NCSA's CM-5, the run used a grid of 134 million zones to produce 70 Giga-bytes of data, according to Norman.

The research is part of the Grand Challenge Cosmology Consortium, a multiuniversity collaboration studying the formation of galaxies in cosmologically large-scale structures. It is funded by NSF's HPCC Initiative [see *access*, Spring 1994]. ▲



NCSA Research Scientist Mike Norman.

(Photo by Thompson-McClellan Photography)

NCSA RealTime: Time to go digital

by David Curtis, NCSA Creative Director, Scientific Communications, and Executive Producer, NCSA RealTime

Just over three years ago NCSA launched *NCSA RealTime*, the first general interest video magazine reporting on HPCC. Covering a wide range of topics from science and engineering to the arts and humanities, the video magazine's six editions were seen extensively.

As a proof-of-concept, *NCSA RealTime* demonstrated that it was possible to communicate computational science and engineering themes to diverse audiences through broadcast-quality video stories. Reaching large numbers of viewers via cassette, satellite, broadcasts, and cablecasts in the U.S. and Japan, the program helped to spur TV producers at PBS, ABC, and CNN to create their own news and documentary programming on computational science and scientific visualization.

However, for NCSA, the rapid pace of convergence in digital video, computing, and telecommunications technologies points to the need to develop new, interactive channels of distribution for video programming.

As part of a strategic realignment of its creative and technical capabilities focused on outreach, NCSA will cease producing *NCSA RealTime* as a half-hour linear program. Instead it will create short, digitally compressed video stories with the latest desktop computer tools. Using NCSA Mosaic, these stories will be integrated with explanatory text and scientific imagery and then linked to the wealth of online information already available on servers at NCSA and elsewhere. The resulting cyberspace programming will be an innovative multimedia resource for anyone on the Internet.

NOTE: Cassettes of the six editions of *NCSA RealTime* are available for purchase. For ordering information, contact Orders for Publications, NCSA Software, and Multimedia [see *nscs contacts*, page 2]. ▲

Truth continued from page 16

Critical insight

The consensus of the panel was that online hypermedia holds great promise for developing presentations that combine narrative, sequential videos with a rich, in-depth database. (An example is the CD-ROM presentation accompanying the book by Robert Wolff and Larry Yaeger that is reviewed on page 25.) While information design issues continue to be important, context, use, and intent must be considered when evaluating scientific images.

Finally, it was determined that education and training of producers and consumers of scientific imagery will enhance critical thinking about scientific images. ▲

References

1. N. Oreskes et al, "Verification, Validation and Confirmation of Numerical Models in the Earth Sciences." *Science* 263: 641-646 (February 4, 1994).
2. *Ibid.*
3. "Theory Center Visualization." *Frontiers* 9:1 (Summer 1993).
4. Quote from *Numerical Methods for Scientists and Engineers* by R. W. Hamming (New York: Mc Graw-Hill, 1962). Note: The 1973 edition is prefaced with this variation of the quote: "The purpose of computing is not really in sight [sic]."



Jarrett Cohen, former NCSA staff associate in the Director's Office, is now a Senior Publications Specialist at the NASA/Goddard Space Flight Center in Greenbelt, MD. (Photo by Tony Baylis, USEO)

Bushell at SIGGRAPH 94

NCSA Research Programmer Colleen Bushell (SDG) was a member of the "Information Visualization: The Next Frontier" panel at SIGGRAPH 94.

Nahum D. Gershon of The MITRE Corp. was panel chair. Other members were Jock D. Mackinlay, Xerox Palo Alto Research Center; William A. Ruh, The MITRE Corp.; Anselm Spoerri, MIT; and Joel Tesler, SGI.

Panel members and the audience discussed the use of data visualization methods, software, and hardware in presenting abstract information contained in databases, digital libraries, and other extensive collections of data and information. The panelists and the audience discussed how to create effective visualizations and how to use them in information navigation, retrieval, and access in the information highway environment.

In her presentation, Bushell cited examples of communications with complex data and information that incorporate visual, qualitative representations and quantitative data—e.g., scientific visualization, interface design, cartography. Ideas for future features of NCSA Mosaic and suggestions for the graphic design of "home pages" were presented. ▲



NCSA's Software Development Group (SDG) was awarded *InfoWorld* magazine's 1993 Industry Achievement Award for NCSA Mosaic. Receiving the award from Publisher Bob Metcalfe were (left to right) Terry McLaren, Chris Wilson, Tom Redman, Kim Stephenson, and Susan Goode. Dave Thompson was not present. These SDG members represent all three platforms (Macintosh, Microsoft Windows, and X Window System) and technical support of the development team. (Photo by Wilmer Zehr Photography)

Ars Electronica award winners by Fran Bond, Editor

European artists Christa Sommerer and Laurent Mignonneau, participants in NCSA's Fine and Applied Art Visitors Program for the 1993-94 academic year [see *access*, Spring 1994], recently traveled to the Ars Electronica Festival at Linz, Austria, to receive the distinguished Prix Ars Electronica 94 Golden Nica in Interactive Art. Their award-winning work, *A-Volve*, was developed during their association with NCSA. For it, they won \$16,000 (U.S.).

Viewers of Sommerer and Mignonneau's artwork interact with virtual creatures in a water-filled glass pool as they design shapes and profiles on a computer monitor with a sensor pencil. Algorithms developed by Sommerer and Mignonneau ensure that the creatures "swim" smoothly.

Ars Electronica, Europe's largest festival of art and technology, is a yearly competition that awards prizes in four categories: animation, graph-

ics (images), music, and interactive art. This year there were a record number of 1,584 entries from 38 countries. The competition, ongoing since 1987, was organized by Austrian Television, endowed by the Kapsch Co., and sponsored by the City of Linz and the Province of Upper Austria.

SIGGRAPH 93 was the locale of the first U.S. showing of the artists' work. Previous joint exhibitions were in Austria, France, Germany, Finland, and Switzerland. In February 1994, they were invited to participate in *Imagina 1994* at Monaco and show *Interactive Plant Growing*.

Early in July, the artists left for Tokyo to develop an interactive art project for Nippon Telephone & Telecommunications (NTT), which will be shown at NTT's InterCommunications Center, a museum of art and technology scheduled for opening in 1996. Bon voyage! ▲

abbreviations

ANL	Argonne National Laboratory
ARPA	Advanced Research Projects Agency
CTC	Cornell Theory Center
DoE	Department of Energy
HPCC	High Performance Computing and Communications
NASA	National Aeronautics and Space Administration
NCAR	National Center for Atmospheric Research
NCSA	National Center for Supercomputing Applications
NII	National Information Infrastructure
NSF	National Science Foundation
PSC	Pittsburgh Supercomputing Center
SDG	Software Development Group
SDSC	San Diego Supercomputer Center
SGI	Silicon Graphics Inc.
TMC	Thinking Machines Corp.
UIC	University of Illinois at Chicago
UIUC	University of Illinois at Urbana-Champaign
URL	Uniform Resource Locator
VEG	Virtual Environments Group

documentation orders

Articles in this *access* may refer to items that are available through the *NCSA Technical Resources Catalog*. To receive a copy of the catalog, send your request to Orders for Publications, NCSA Software, and Multimedia [see *nscs* contacts, page 2].

accessing NCSA's servers

Many NCSA publications (e.g., calendar of events, user guides, *access*, technical reports) as well as software are available via the Internet on one of three NCSA servers: anonymous FTP, Gopher, or the World Wide Web. If you are connected to the Internet, we encourage you to take advantage of the easy-to-use servers to copy or view files.

NOTE: NEW Anonymous FTP IP address: <ftp.ncsa.uiuc.edu> (141.142.3.135)

Gopher server IP address: <gopher.ncsa.uiuc.edu>

World Wide Web IP address: www.ncsa.uiuc.edu

NCSA WWW Home Page: <http://www.ncsa.uiuc.edu/General/NCSAHome.html>

NOTE: References in *access* to a World Wide Web URL (Uniform Resource Locator) refer to the server address and file location information used by NCSA Mosaic software to retrieve documents.

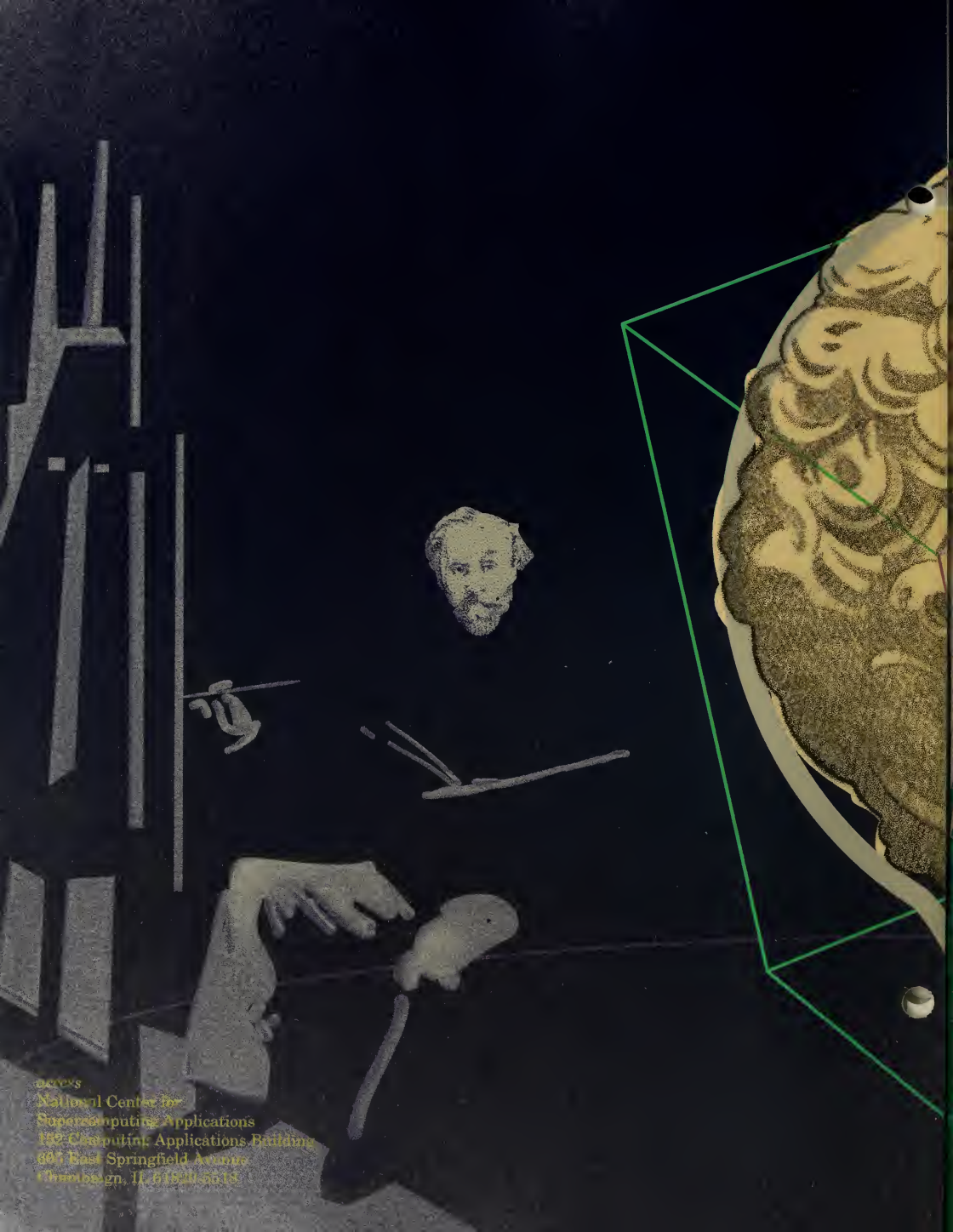
If you have any questions about accessing the servers, contact your local system administrator or network expert. Instructions for accessing the anonymous FTP server follow.

downloading from anonymous FTP server

A number of NCSA publications are installed on the NCSA anonymous FTP server. If you are connected to Internet, you can download NCSA publications by following the procedures below. If you have any questions regarding the connection or procedure, consult your local system administrator or network expert.

1. Log on to a host at your site that is connected to Internet and running software supporting the FTP command.
2. Invoke FTP by entering the Internet address of the server: `ftp ftp.ncsa.uiuc.edu` or `ftp 141.142.3.135`
3. Log on using `anonymous` for the name.
4. Enter your local login name and address (e.g., `smith@ncsa.uiuc.edu`) for the password.
5. Enter `get README.FIRST` to transfer the instructions file (ASCII) to your local host.
6. Enter `quit` to exit FTP and return to your local host.
7. The NCSA publications are located in the `/ncsapubs` directory.

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departments

- 2 ncsa contacts
- 3 editor's note
- 24 center activities
- 28 book review



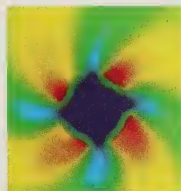
Cover: The quest for a teraflop computing engine is as challenging as conquering great mountains.

Cover produced on a Macintosh IIfx using Adobe Photoshop, Aldus FreeHand, and a UMAX UC630 scanner. (Concept and illustration, John Havlik; concept and research, Fran Bond)

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A

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Fall 1994

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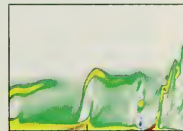
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research

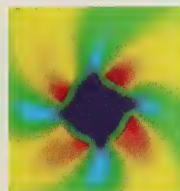
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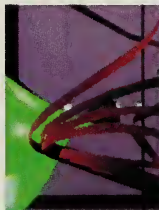
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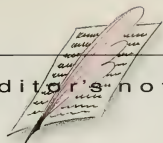
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NOTE: All electronic mail addresses are via Internet.

See inside back cover for details on anonymous FTP, Gopher, and World Wide Web.



Along the pathway on the search for more sophisticated computing engines, NCSA is positioning for the next generation of HPCC. Currently the center is integrating scalable microprocessing machines into its metacomputing environment. These changes are outlined in "Scalable metacomputing strategy at NCSA" on page 4. An analysis of this strategy, "NCSA assesses application codes," can be drawn from scalability studies conducted at the center (see page 6).

NCSA's new configuration of scalable architecture includes the retirement of the vectorized CRAY Y-MP system. For a survey of significant science produced on that machine, turn to page 9.

Read about how UIUC students in a dynamic modeling class learned the principles of computational modeling in "Modeling impacts the environment" (page 12). "Data driven sound: The next step" (page 14) describes the addition of sonification to scientific research utilizing NCSA's virtual environment. Last summer high school science and math teachers became students again in a new version of SuperQuest (see "NCSA sponsors SuperQuest for Teachers" on page 17).

In the new technology section, various aspects of NCSA Mosaic's impact are presented, including some helpful advice on "HTML for World Wide Web users" (page 20) and an online state fair (page 23). Examples of the center's outreach, including CCNet activities (page 24) and training local high school students to make a documentary (page 25) may be found in the center activities section.

Howard Rheingold's latest book, *The Virtual Community: Homesteading on the Electronic Frontier*, is reviewed on page 28.

—Fran Bond, Editor



"People who might say 'Who needs petaflop computing today?' are the same folks who asked who needs a teraflop, who needs a gigaflop, who needs a megaflop. The automation of activities of society, of industry, and of government will never end."

—George Cotter, U.S. National Security Agency, quoted in *High Performance Computing and Communications Week* (September 1, 1994).

Scalable metacomputing strategy at NCSA

Adapted from a report by NCSA Computer Policy Committee; John Towns, Chair

Illustrations by John Havlik

This year NCSA is moving to a set of computational systems based solely on microprocessors. Such systems offer excellent performance, are compatible in an applications and programming environment with popular desktop systems, and offer the most economically viable path toward achieving a teraflop in sustained performance by the end of the decade.

In response to evolving conditions in technology and government funding, a group of research scientists, applications and system programmers, and networking experts developed a plan for NCSA to acquire major computational systems over the coming years. A report entitled "The NCSA Scalable Metacomputing Strategy" (April 1994) summarizes the strategy and justification for system acquisition and upgrades and presents details about the features and arrival dates for those systems.

The driving force behind this change is the federal government's HPCC effort (summarized in "High Performance Computing and Communications: Technology for the National Information Infrastructure" and "High Performance Computing and Communications: Toward a National Information Infrastructure") that looks to achieve a sustained teraflop computing performance capability by the end of the decade. [1] NCSA is taking an aggressive approach to achieve this goal by acquiring early systems, supporting the development of applications, and pushing the mechanisms that will fund and support a teraflop system(s).

For the next two years, NCSA is committed to providing access to large parallel systems that employ both distributed memory and shared memory implementations. A variety of strategies for migration of applications to these systems are being actively investigated today. NCSA will assist each user in identifying the most appropriate architecture for his/her application.

NCSA solicits your questions, comments, and suggestions on this strategy. Send them via email to future@ncsa.uiuc.edu (Internet).

NCSA research

Since 1991 NCSA has conducted an exhaustive analysis of the performance of an ensemble of national user applications on the center's 4-processor Cray Research Y-MP. The results show that

- all but a small percentage of users compute on single processor vector nodes,
- the average code runs at 25% of peak speed of that single vector processor—which is ~80 megaflops (Mflops) on the CRAY Y-MP system, and
- two-thirds of NCSA's users run below this speed.

In the large mix of high-performance users, scalar code usage seems to dominate.

Over this same period, many changes have occurred in high-performance systems. A new performance curve has evolved—with RISC and superscalar technologies showing much faster gains in performance than traditional vector supercomputer processor advancements. Concurrently, advances and techniques have developed for networking of these smaller compute nodes into parallel systems with varying degrees of parallelism. Both distributed and shared memory implementations have been developed. Because of these changes and technological advances, NCSA sees its mission as that of assisting the majority of users to achieve a major increase in performance by moving their applications to highly parallel systems made up of the fastest RISC superscalar processors available.

In preparation for this move, NCSA staff have worked for four years on distributed memory microprocessor equipment [CM-2 and CM-5 plus IBM and Hewlett-Packard (HP) workstation clusters]. Our studies indicate such a distributed-memory architecture is quite appropriate for those codes not requiring extensive load balancing or interprocessor communication. This has allowed many applications to move to departmental-scale clusters, while over 100 projects are currently running on the center's 512-node CM-5. (See Figure 1 on page 7.)

More recently, NCSA has been investigating shared-memory architectures with a 32-processor SGI Challenge XL and an 8-processor CONVEX Exemplar. Shared memory multiprocessors offer much faster interprocessor communications via high-speed memory backplanes and allow very good performance and high efficiency, but these systems do not currently scale to as many processors as the distributed memory machines.





TERAFLOP

NCSA's goal is to continue to aggressively expand its capacity over the next few years. Specific acquisitions and other details for this year are noted below.

SGI

An SGI Challenge multiprocessor became available in May 1994. This machine has 32 R4400 processors (150 MHz, 75 Mflop peak), 2 Gbytes of shared memory, and 80 Gbytes of RAID disk. In November 1994, it was upgraded to a Power Challenge R8000 with 16 superscalar processors, each running at 75 MHz and 300 Mflop peak speed and each with 128 Mbytes of RAM. This machine will be binary compatible (for single processor applications) with R4000-, R4400-, and R4600-based SGI workstations.

In addition, NCSA is experimenting with a Houston-based SGI Challenge Array consisting of four networked Challenge machines with 20 processors each. This array will be used to evaluate high-performance science and engineering applications as well as its applicability as an information server for digital library and multimedia applications.

Convex

NCSA acquired a CONVEX Exemplar hypernode on April 22. The hypernode consists of 8 processors, with a peak speed of 200 Mflops per processor and 512 Mbytes of shared memory. It is binary compatible (for single processor applications) with HP 735 workstations. This machine is expected to be available for friendly user access in the last quarter of 1994.

Plans are in place, pending funding approval, to upgrade this machine to 8 nodes (64 processors) with 4-Gbytes total memory and 80 Gbytes of RAID disk. The current 8-processor vector architecture C3880 system is scheduled to be removed from service when the single hypernode Exemplar system is in production mode. The Exemplar presents the user with a cache-coherent shared memory programming environment and will be a good candidate architecture for many of the smaller CM-5 users.

Thinking Machines

NCSA has retained the current 512-node CM-5 system. The CM-2 was retired May 2, 1994. NCSA plans to continue using the CM-5 for the natural life of the machine. (See Thinking Machines Corporation's recent statement to CM-5 users on page 8.)

Migration strategy

In moving to microprocessor-based parallel systems, NCSA is adopting an aggressive strategy that includes removing the traditional vector platforms (CRAY Y-MP and CONVEX C3880 systems) later this year. The National Metacenter (the four NSF supercomputer centers plus NCAR) offers a variety of machines that will continue to be available for use on a peer review basis. NCSA encourages you to consider the following factors and suggestions in evaluating future platforms for your applications.

NCSA's commitment

From an applications development point of view, we have observed that most applications optimized for vector processors also become good performers on superscalar workstation-level machines. This is particularly true on the next generation microprocessors such as the SGI Power Challenge R8000. (See Figure 2 on page 7.) In addition, users require the standard programming languages including FORTRAN 77 with Fortran 90 extensions, C, and C++. Industrial users require a wide spectrum of supported, third-party applications.

With this in mind, a further goal is to move toward systems that offer binary compatibility with desktop machines to facilitate development and analysis phases of a research effort to be performed at the user's local site. This strategy also ensures that the maximum number of third party codes will be available.

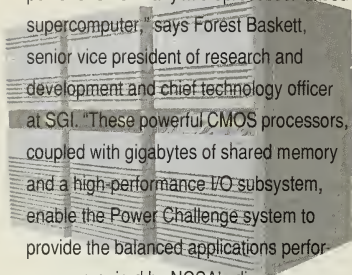
NCSA's upgrade strategy

NCSA will remove its traditional vector machines by December 31, 1994 (CRAY Y-MP and CONVEX C3880), leaving machines based solely on microprocessor hardware. The center will utilize microprocessor-based systems from three vendors: Silicon Graphics Inc. (SGI), Convex Computer Corporation, and Thinking Machines Corporation. A 16-processor SGI Power Challenge machine was installed in November 1994, a CONVEX Exemplar 8-processor hypernode was installed in April 1994, and the Thinking Machines CM-5 is being retained.

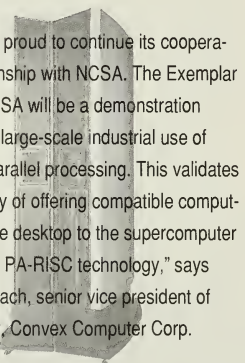
Vector platform users

The vast majority of NCSA's Y-MP projects could receive more cycles and similar turnaround on dedicated workstations (see Figure 1). The Branscomb Report to the NSF ("From Desktop to Teraflop: Exploiting the U.S. Lead in High Performance Computing"), currently under review by the National Science Board, recommends the provision of \$20 million for such workstations. [2] NCSA can provide support for project proposals seeking to acquire workstations by

Scalable continued on page 7



"The R8000 RISC processor is the most powerful CPU in any microprocessor-based supercomputer," says Forest Baskettt, senior vice president of research and development and chief technology officer at SGI. "These powerful CMOS processors, coupled with gigabytes of shared memory and a high-performance I/O subsystem, enable the Power Challenge system to provide the balanced applications performance required by NCSA's diverse community of researchers."



"Convex is proud to continue its cooperative relationship with NCSA. The Exemplar SPP at NCSA will be a demonstration vehicle for large-scale industrial use of scalable parallel processing. This validates the strategy of offering compatible computing from the desktop to the supercomputer using HP's PA-RISC technology," says Steve Wallach, senior vice president of technology, Convex Computer Corp.

"NCSA's homogeneous environment of Silicon Graphics equipment will be unique," says NCSA Director Larry Smarr. "Tightly integrating desktops, classrooms, virtual reality, and supercomputing will allow new levels of insight into the simulation of complex dynamic systems.

"We see the CONVEX Exemplar as a crucial step in allowing corporate America to reap the benefits of parallel computing. Our goal is to have the largest shared- and distributed-memory machines in the NSF Supercomputer Centers Program. The Exemplar and the CM-5 will provide our users with such resources," says Smarr.

NCSA assesses application codes

by Michael Welge, NCSA Technical Program Manager, Applications Group

For several months, NCSA has been conducting scalability studies and cross-architecture comparisons of a number of academic and third-party applications codes in its multivendor scientific computing environment. The purposes of this effort are (1) to evaluate the effectiveness of various parallel architectures for large-scale scientific computing, (2) to determine the level of effort required to port realistic-sized codes to parallel environments, and (3) to determine the extent to which portability is achievable across diverse architectures (and at what price to performance ratio).

This project has focused on three major parallel platforms already in place at NCSA: the Thinking Machines CM-5, the CONVEX Exemplar, and the SGI Power Challenge. These three machines represent three major architectural paradigms: pure distributed memory, distributed memory with a global address space, and pure shared memory, respectively. Although NCSA's efforts will naturally continue to focus primarily on machines in-house, the center would expect to expand the list of architectures used through collaboration with other institutions.

Since much of the production work of NCSA's industrial users relies on third party application codes, we have initiated a new program to evaluate the most heavily used third party codes on NCSA's various architectures. Nine application teams have been created, one for each of our partners' most widely used application codes (ABAQUS, CHARMm, FIDAP, Flow3D, FLUENT, Gaussian, KIVA, NASTRAN, and Spectrum). Each team is anchored by an appropriate NCSA applications scientist and contains volunteers from among the largest partner users. So far, there are 16 strategic user volunteers signed up from six of NCSA's industrial partners. These teams will create nonproprietary, but relevant, application datasets of varying sizes, so that the scalability of each application code can be assessed. The results of these runs, made during the next six months, will be made available to NCSA's partners. For details, see the NCSA Application Performance Home Page on the World Wide Web via NCSA Mosaic (see URL below).

In a similar manner, NCSA has called upon its academic research user community to collaborate in exploring and understanding the scalability of these systems as applications move from a single to hundreds of processors. Currently, there are efforts in the areas of astrophysics, biology, chemistry, earth sciences, gravitation, fluids, and structures. The goal is to optimize the working environment for users and to determine the most appropriate upgrade strategy for the future.

NCSA has also invited various computer vendors to collaborate in this effort. The initial focus has been on the SGI Challenge, as it offers the most mature development environment at present. With the arrival of the CONVEX Exemplar and upgrades to the operating system and processors of the SGI Challenge, our efforts will be expanding to these new systems. ▲

NCSA Application Performance Home Page:
http://www.ncsa.uiuc.edu/Apps/perf/NCSAperf_homepage.html

SGI Power Challenge (top), CONVEX Exemplar, and Thinking Machines CM-5 (bottom). (Photos by Wilmer Zehr Photography)

offering time for porting and benchmarking activities on SGI and HP systems.

For many applications, it is now possible to run on a workstation at similar or higher performance than the CRAY Y-MP, as shown in early results from the SGI Power Challenge. (See Figure 2.) For example, one 17-Mflop run of ABAQUS on the Y-MP achieves 21 Mflops on a single processor of the SGI Power Challenge. Parallelizing these codes on the SGI Challenge or CONVEX Exemplar can then potentially yield a few to tens of times speedup relative to single vector processor performance. (The higher speedup depends on the planned 64-node CONVEX Exemplar anticipated in late 1994.)

For highly vectorized codes, users are encouraged to begin evaluating parallel systems immediately. These systems will continue to offer greatly enhanced performance for many applications, as well as increased memory over the current set of vector architecture machines available. (See related article on page 6.)

NOTE: If your migration process requires the use of a vector multiprocessor beyond December, CRAY C90 vector machines are available through peer review at SDSC and PSC.

Again, please send any questions or comments about this plan to future@ncsa.uiuc.edu (Internet).

References

1. These Blue Book Reports may be obtained from the National Coordination Office for High Performance Computing and Communications, Bldg. 38A/B1-N30, 8600 Rockville Pike, Bethesda, MD 20894. They are also available via the WWW at the URL given below.
2. This may be obtained as Report NSB 93-205 from NSF at the National Science Foundation, Arlington, VA 22230. The report is also available via the WWW at the URL given below and via Gopher at gopher://stis.nsf.gov/00/CISE/reports/nsb93205 ▲

NCSA Project Usage: FY94

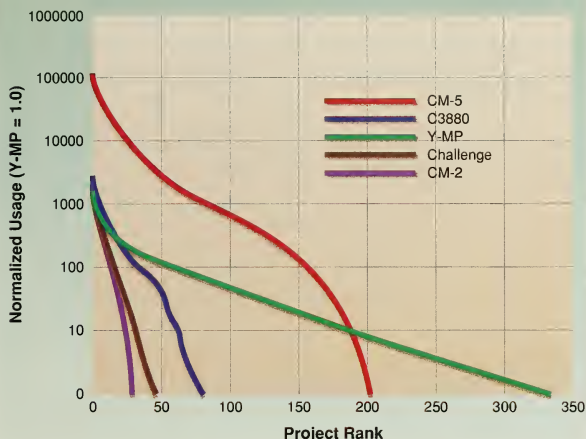


Figure 1. NCSA project usage on machines in FY94. (Courtesy of Lex Lane; illustration by Marshall Greenberg)

SGI Power Challenge vs. CRAY Y-MP



Figure 2. Performance on NCSA's Power Challenge (R8000) system compared with CRAY Y-MP system. (Courtesy of Michael Welge; illustration by Marshall Greenberg)

Blue Book Reports: <http://www.hpcc.gov>

The Branscomb Report (NSB 93-205): <http://www.hpcc.gov/reports>

To the worldwide Connection Machine Users Group

EDITOR'S NOTE: The following message was sent to members of the CM-5 User Group from executives at Thinking Machines Corp. in late August. This message has been posted online on NCSA's systems.

We would like to update you on the current situation at Thinking Machines and the progress we are making on rebuilding our company.

As you may have heard or read, . . . our Board of Directors decided to apply to the courts for protection from our creditors under Chapter 11 of the U.S. Bankruptcy Code in order to give us time to redirect our business strategy. This was a difficult decision but one that was unavoidable given the current state of the supercomputer market and our desire to be in position to continue to serve our customer base. We believe that the company, once we reorganize and readjust our cost structure, cannot only survive but become a thriving and profitable business. Chapter 11 allows us the time and protection to achieve this. Our goal is to develop and implement a new business plan as quickly as possible in order that we reemerge from Chapter 11 at the earliest possible time.

We have already begun restructuring our business to focus on our existing customers and to exploit our considerable and acknowledged leadership in parallel systems and parallel software technology. As part of this reorganization, . . . we took the necessary but very painful step of dismissing one-third of our work force. This action, which was required to bring our costs into line with our current revenues, will have minimal effect on the contracted services we provide to our installed base.

We have three key priorities which will be the foundation of the business plan:

CRAY CS6400 to arrive in 1995

National information servers for spatial data analysis systems and environmental data are being established at NCSA and SDSC. These machines will be linked to existing servers for atmospheric information and NASA remote sensing data.

In January 1995 NCSA will begin an evaluation of a CS6400 (CRAY SUPERSERVER 6400) system. Information-serving applications for this architecture include digital libraries, geographical information systems (GIS), and WWW servers.

The CS6400 is a SuperSPARC-based symmetric multiprocessor system targeted at information serving/processing applications. It is the high-end system in a series of server systems by Sun Microsystems. The CS6400 can be configured with up to 64 processors and 16 Gbytes of memory.

Plans are underway for a multidisciplinary, multiscale program that will aid in the analysis of landscape dynamics and exploration of options in resource management. By developing a nationwide resource for spatial data analysis on the new server, a new category of natural users—from the research community and the public—will have access to comprehensive data and simulations.

1. Support our existing customer base.

We will continue to provide our customers and their users with the same high quality of support services that has set the standard for the industry, both from the Home Office staff in Cambridge and from our extensive U.S. and international field operations. We have the resources in place to provide this service and support now and in the future. Our relationship with our customers is among our most prized assets. We intend to work very hard over the next few weeks and months to reaffirm the close working relationships that we have enjoyed with so many of you in the past.

2. Continue to offer CM-5E systems.

We will continue to offer CM-5E systems, upgrades, and expansions to our existing customer and prospect base. We have the inventory and production capability to supply this equipment, and we are actively pursuing such opportunities. Our plans are to provide a clear software upgrade path for our existing Connection Machine customers.

3. Offer Thinking Machines parallel software on other parallel platforms.

We expect to be consolidating and refocusing our resources to make our suite of parallel system software available on high-volume parallel platforms from other vendors. This is a key area of opportunity for the company and builds on the reputation we have earned for providing the most complete and sophisticated parallel computing software environment in the world.

We ask for your patience and understanding, especially in the next few weeks, as we go through this period of adjustment. Our relationship with you is critical to the nature of this company, and supporting you remains of paramount importance to each and every employee of Thinking Machines. We have appreciated your critical advice and encouragement in the past and hope you will continue to provide us with this input and support through the present transition period into the future. We are confident that over the coming months we will be able to provide you with a range of exciting products and services that will be consistent with and supportive of your long-range development and production application strategies. Our plans are to be at Supercomputing '94, so we look forward to seeing many of you there.

Dick Clayton, President

Dale Fisher, Director of Customer Support

David Lloyd Owen, European Manager, Customer Support



CORNUCOPIA OF CRAY Y-MP SCIENCE

BY KENNETH CHANG, GRADUATE STUDENT AT THE UNIVERSITY OF CALIFORNIA, SANTA CRUZ;
FORMER NCSA RESEARCH PROGRAMMER, PUBLICATIONS GROUP

In November 1990, NCSA's CRAY Y-MP4/464 computer system went into service. By the time it is retired later this year, over 6,200 researchers and their students will have performed more than 100,000 hours of calculations on its four processors.

The machine's speedy floating point performance, coupled with copious memory and disk resources, allowed scientists to explore problems in astrophysics, chaos, chemistry, materials science, and other areas that were previously out of reach.

"The Cray Research Y-MP product line enabled more supercomputing science and engineering projects than any computer in history," NCSA Director Larry Smarr says.

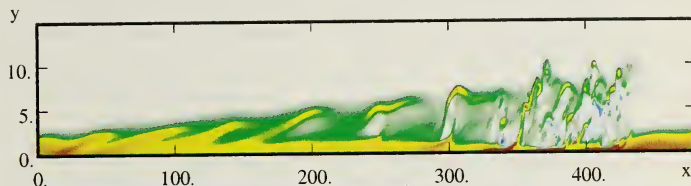
A quick survey of a number of projects performed on NCSA's Cray Y-MP system follows.

Chaos and turbulence

Watch smoke rise from a cigarette. Initially, white wisps rise smoothly and evenly from the burning tip. Higher up, the flow begins to falter and then disintegrate into a tangled turbulence of whorls and eddies. The equations that describe the process—the Navier-Stokes equations—can be written in a few lines of mathematical notation. Solving the equations beyond a few simple situations, however, remains one of the most intractable of scientific problems.

In the 1970s, a theory called "secondary instability" attempted to explain how fluids become turbulent. Although that theory is successful in some cases, it does not agree with data from other experiments.

Dan Henningson, formerly at MIT and now a mechanics professor at the Royal Institute of Technology in Sweden, and Satish Reddy, mathematics professor at the Univer-



Streamwise shear in a wall normal symmetry plane showing the intensification and breakdown of shear layers (yellow tongues surrounded by green). Reynolds number at the inflow is $R=400$, based on free-stream velocity and displacement thickness. Blue, green, yellow, to red color coding shows regions with the low to high values of shear. (Courtesy of Dan Henningson from Berlin, Lindblad, and Henningson in *Phys. Fluids* 6:1949-51, 1994)

sity of Oregon, have been exploring an alternate theory called the bypass transition. Because of friction, particles flowing next to a wall move slower than those further away. If a pocket of fluid is disturbed such that it moves further from the wall, it collides with faster-moving particles. (Similarly, a pocket that moves towards the wall collides with slower-moving particles.) Until supercomputers, scientists could not determine whether these disturbances snowball into chaos or just damp out, preserving the smooth flow.

"Numerical simulations [on the Y-MP] have been able to follow these types of disturbances during the complete transition process into the turbulent regime," Henningson says. "The simulation showed once you have these streaky structures, they began to bend like a snake back and forth and then quickly break down into turbulence."

At least in certain cases, bypass transitions require just 1/100 to 1/1000 of the energy required by

secondary instabilities to cause the transition to turbulence.

The dynamics of combustion are even more complicated than those of fluid flows, because of additional equations governing the chemical reactions of burning fuel. Until recently, the best that could be done was to take a statistical look at average temperatures, velocities, and pressures within.

The processing power of the Cray Y-MP allowed Peyman Givi, professor of mechanical and aerospace engineering and director of the Computation Fluid Dynamics Laboratory at the State University of New York-Buffalo, "to attack these equations directly and solve the problem by brute force."

Even though relatively simple simulations still require more than 200 hours of computing time each on the Y-MP, Givi's "direct numerical simulations" have provided more

CRAY-MP continued on page 10

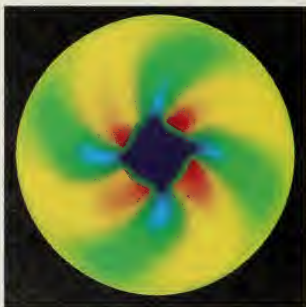
detail than previously possible about the workings of turbulent combustion devices—from scramjets to boilers to car engines.

"The data, we claim, are more accurate than experiments because we have exact control over the system," Givi says. "We know exactly what is going on in the engine at every point at all instances—something experimentalists cannot claim."

To benefit engineers who design combustion devices, Givi and his coworkers condensed this wealth of numerical data down to mathematical models. "We have come up with simple equations that can be run on a calculator," he says.

Consider a point source of combustible gaseous mixture in 2D. When the temperature becomes sufficiently high, chemical reactions leading to combustion occur. A flame front separates the fresh mixture from the combustion products.

The flame front would like to propagate inward to consume the unburned gas, but is pushed back by fresh mixture emanating from the source, so that an equilibrium is achieved. The simplest situation occurs when the front is circular with uniform temperature. This is the model **Alvin Bayliss** and **Bernard Matkowsky**, professors of engineering science and applied mathematics at Northwestern University, use to explore pattern formation in flames.



Color coded visualization of cellular flame. Flame shown is a modulated traveling wave in which the cells change shape and speed as they rotate. (Courtesy of Alvin Bayliss and Bernard Matkowsky)

They are interested in the formation of cellular patterns in flames. Cells can be thought of as wrinkles along the front in which hot regions alternate with cooler ones. Cellular behavior depends on the *Lewis number* (Le)—the ratio of thermal to mass diffusivity of the limiting reactant of the mixture. For Le near 1, no cells form. As Le is varied, transitions to a rich variety of cellular flames occur. These include stationary cells, traveling waves (where cells rotate uniformly like a pinwheel), modulated traveling waves (where cells change shape and speed as they rotate), and chaotic flames (where cells are randomly created and annihilated). Chaotic flames represent the simplest of turbulence in combustion.

These numerical studies may eventually have applications to controlling combustion. For now, the primary purpose is "to understand the transition from laminar to turbulent combustion," Bayliss says. Experiments have demonstrated patterns qualitatively similar to the computations.

Materials science

Under normal circumstances on the Earth's surface, the air around us exerts a pressure of about 14 pounds per square inch. By pressing two diamonds together, scientists can now achieve pressures of up to *tens of millions* of pounds per square inch—roughly what one finds at the Earth's center.

Not surprisingly, materials behave quite differently under extreme conditions. Using a model developed to describe the behavior of crystalline solids—materials where atoms are positioned on a precise, repeating lattice, like a pattern of floor tiles—University of California, Berkeley Physics Professors **Marvin Cohen** and **Stephen Louie** have explored some of these possibilities via simulations on the CRAY Y-MP.

"We try to produce new materials on the computer," Cohen says. His model was the first to incorporate fundamental interactions in atoms; an earlier model had relied on properties derived from experimental data.

For example, at normal pressures silicon is a semiconductor. Cohen's and Louie's calculations predicted that at high enough pressure, silicon would reshape itself into a hexagonal form and be transformed into a

superconductor. Experiments have since verified this prediction.

Because materials sometimes retain their transformed structure, even after high pressures are removed, this process may eventually have important technological applications, especially in producing semiconductors. Cohen says that "you can tailor these materials" to fit specifications for various devices, such as lasers or solar energy panels. "You can make some of these strange things we are proposing."

Quantum mechanics has been successful in explaining the behavior of atomic and subatomic particles. Applied to larger objects such as molecules—which can consist of hundreds or thousands of atoms each—the full equations of quantum mechanics quickly become unmanageable, however.

David Coker, chemistry professor at Boston University, has approached this problem by carving it into two pieces. Coker's algorithm, *nonadiabatic dynamics*, first solves for the quantum mechanical behavior of lighter, faster moving parts of a molecule. The calculated forces are then coupled to the motion of the molecule's heavier parts, which can be solved by older, simpler Newtonian classical dynamics.

"The trick is finding the most accurate and efficient way to break the system into heavy and light parts so that you do as little quantum mechanics as possible," Coker says.

Most earlier simulations of molecular dynamics did not include quantum effects and "were usually done on the ground state of the molecule," Coker says. These calculations could not describe phenomena such as the breaking of chemical bonds or photochemistry, where reactions are stimulated by shining light on chemicals.

One application of Coker's methods may be in the engineering of optical devices. By diffusing hydrogen molecules into a glass fiber and then inducing reactions between the hydrogen and surrounding silica molecules with laser pulses, researchers hope to precisely manipulate the fiber's optical properties. Using nonadiabatic dynamics—here, the "light" part of the problem is the rotational motion of the hydrogen molecules—

Coker calculated how hydrogen diffuses within the optical fiber.

These fibers may be an important step toward optical computers. "Just as a transistor controls the flow of electrons, an optical fiber with tailored optical properties can control the flow of photons," Coker says.

Nonadiabatic dynamics is much more general, however, and "can be applied to anything that involves excited state dynamics, such as the plumes of rocket engines," he says.

Biophysics

Twenty naturally occurring amino acids form a kind of alphabet of life. These organic molecules, which are strung together in chains ranging typically in lengths from 50 to 500, are the amino acids that form a vocabulary of proteins—the basic building blocks for animals and plants.

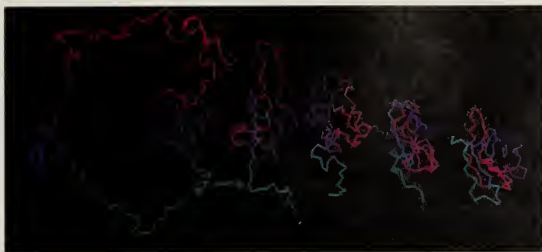
The sequence of amino acids in a protein—essentially its "spelling"—does not fully define the protein's meaning. Initially a spaghetti-like strand, a protein quickly folds up into a rigid, almost crystalline structure, and this structure largely determines its chemical properties and functions.

"It's only the folded protein which really has the information organized such that the molecule can function," says **Peter Wolynes**, UIUC chemistry professor. "Until we understand how the sequence is translated into structure, there is a missing link in our understanding of how information flows in living organisms."

While chemists have been able to determine the sequences of several hundred thousand proteins, they know the structure of only several thousand. Wolynes and **Zan Schulten**, lecturer in UIUC's chemistry department, are using the Cray system to calculate a protein's structure from its amino acid sequence.

By examining proteins with known structures, they develop energy functions that optimize the interactive forces between different amino acids. They then use these approximated forces to simulate the folding process of other proteins.

Recently, they published a prediction, which experimentalists are currently attempting to verify [see *access*, Fall 1993], for the structure of the protein that binds to estrogen and which may play an important role in breast cancer and other diseases.



Snapshot of six stages in protein folding dynamics, showing only the alpha-carbon backbone. Residues of the protein are colored according to their position along the amino acid sequence composing the protein. The protein part of a human immunoglobulin called the Bence-Jones immunoglobulin, or 1rei for short, is depicted.

(Courtesy of Peter Wolynes, Zan Schulten, and Niles Warren)

Civil engineering

The information superhighway will soon be entering . . . the highways.

With traffic on the highways growing faster than new highways can be built, **David Boyce**, director of UIUC's Urban Transportation Center, offers an alternative approach to the problem of traffic jams—smarter roads.

Boyce and a group of researchers have been working on Advanced Driver and Vehicle Advisory Navigation Concept (ADVANCE), which envisions that someday every car will be outfitted with a veritable multi-media system: computer, video screen, CD-ROM drive, voice synthesizer. All vehicles on the road would radio current traffic conditions to a central Traffic Information Center, which, in turn, would send back information about bottlenecks, accidents, or other problems. Using this information, the on-board computer would then determine the best path to one's destination.

To test the potential of intelligent highways, Boyce ran simulations on NCSA's CRAY Y-MP system. "We developed a rather detailed model that enabled us to make those travel time estimates for five different time periods during the day," Boyce says. The computer model predicted that a fully deployed system with automated vehicles could reduce travel times by 10%.

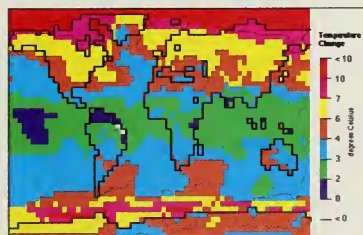
Beginning late this year, the first of 3,000 vehicles will be outfitted with the ADVANCE equipment that was designed by Motorola, one of NCSA's industrial partners. Field tests over a 300-square mile region in the northwest Chicago suburbs are scheduled for 1996.

Climate

Every 100,000 years or so, huge expanses of ice descend from the Arctic Circle, down across North America and Europe to sometimes as far south as the central United States.

Since the discovery of Ice Ages about 150 years ago, many hypotheses have been proposed to explain why they occur. Many climatologists now believe that the rise and ebbs of ice result from changes in the latitudinal/seasonal distribution of sunlight—over tens of thousands of years—caused by precession of the Earth's axis, like a spinning top. (*Precession* is the wobble of the Earth's axis due to the pull of gravity from the Sun and Moon.) Additional causes are variations in the Earth's tilt angle and changes in the orbit's shape to be more or less elliptical.

CRAY-MP continued on page 27



Change in annual-mean surface air temperature resulting from a doubling of the CO₂ concentration. The average global mean temperature increase is 4 degrees Celsius. (Courtesy of Michael Schlesinger and Natasha Andronova)

Modeling impacts the environment

by Thomas Krawczyk, Science Writer

In today's complex world, just about everything is interrelated. UIUC Geography Professor Bruce Hannon and U.S. Army Construction Engineering Research Laboratory (CERL) Senior Scientist James Westervelt are working on computational methods to associate interrelationships in many fields.

From ecology to economics, Hannon's classes in dynamic modeling help students understand the underlying principles of modeling. Last spring, his Advanced Ecological Modeling class simulated the plight of the Desert Tortoise (*Gopherus agassizii*) for Fort Irwin, CA, site of army tank training in the Western Mojave Desert. The Desert Tortoise is both an endangered species and a species considered indicative of desert ecological conditions.

Fort Irwin receives only 7 inches of rain yearly, with temperatures reaching up to 110 degrees Fahrenheit during the summer. Its environment is stable. "General Patton's tank tracks [from World War II maneuvers] are still visible in this area," says Westervelt. To best depict the area on a computer, the fort was divided into a grid of 56 x 56 cells with each measuring 1 square kilometer. Changes in this ecosystem over the course of a century were simulated using a time-step of 1 month.

"The tortoise is a long-lived species, with a life span similar to ours," says Hannon. "So we must run the model for a long time to accurately depict any impact on their lifecycle."

Utilizing STELLA II

Hannon's application of choice is STELLA II, a flexible package for building models of dynamic systems and processes. Developed at High Performance Systems Inc. in Hanover, NH, STELLA II can be used to simulate systems in any setting [see access, October–December 1992]. It provides

the ability to reproduce a particular system using simple, precise mapping language. By defining relationships laid out in the map, simulations can be run to test hypotheses.

"STELLA lets us bring people together who are experts in science, but who may have little or no programming and math experience," Hannon explains. "In our case, 'experts' are represented by teams of students who routinely link out to the pertinent experts around the campus and the nation. The basics of STELLA are so easy to learn that previous programming expertise isn't essential."

Model-building is simplified through STELLA's three-step method in which equations that formulate simulations are automatically generated. In the first stage, called mapping, building-block icons construct a graphical representation of input parameters. In the second phase, called the model phase, the software automatically creates equations that are needed to simulate processes. The simulation, or third step, can be viewed as graphs, tables, or animations.

"The key is to have STELLA as the common language among the people who are putting together the basic cellular model," says Hannon. "You have two choices in modeling software: either everyone can understand and use it, or you must have a modeling guru who works along with the group. The old way was to use a modeling guru, and that leads to what I call a 'cult of the modeler.' I don't care for that approach, because people who participate in the project lose track of their contribution and how it fits into the model. Eventually they lose ownership in the whole model and cease to believe in its results. This new process provides them with an understanding of what they are doing every step of the way, and

they believe in the final output. The experts stay with the process at all times."

Hannon and Westervelt divided the class into small working groups, each building a sector of a larger model that could be run independent of the whole. Group members constructed and tested their part during the week, assembling with the class once weekly to build the full cell model.

Westervelt's Geographical Resources Analysis Support System (GRASS) has been used in models developed in past courses. GRASS is a geographic information interface system. "It is not a database, but a process," says Hannon. "You can make databases with it. It is raster-based, rather than vector-based. While GRASS is public-domain, thanks to Jim, both can be used, depending on the situation." Westervelt is finishing his doctorate in Urban and Regional Planning on the construction of a general modeling environment that allows a seamless connection from desktop computers to an HPCC environment.

Initialization of cells in the Desert Tortoise model required generating a vegetation map with the existing Geographic Information System (GIS) maps of Fort Irwin (including elevation, slope, watershed, roadways, etc.) and 200 random transects of 100 meter length (noting shrubs, grass, cover, etc.). These two types of information were then combined in a back-calculated neural network used to describe the vegetation distribution, by type, across the entire area.

Other collaborators in the Desert Tortoise modeling project are Scott Isard, UIUC Department of Geography; Tony Krzysik, CERL Environmental Sustainability Laboratory; Kevin Seel, Oak Ridge Associated Universities; and Eric Lambert, Illinois State Historical Survey.

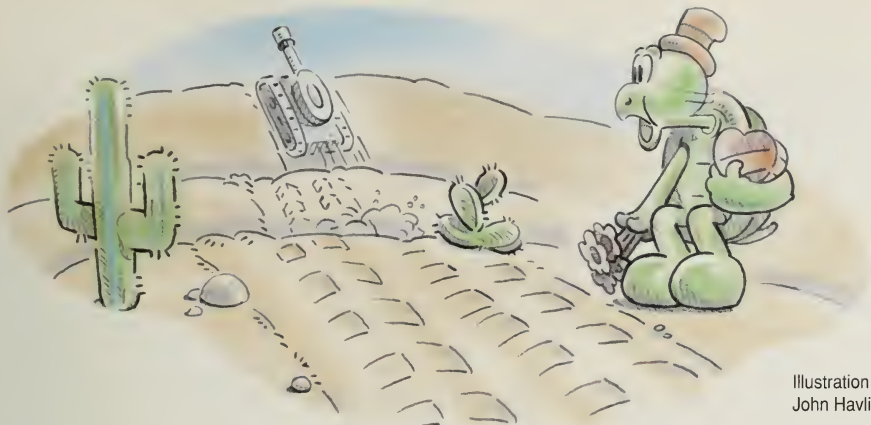


Illustration by
John Havlik

Modeling interrelationships

Advanced modeling methods in the classroom are relatively new. "To my knowledge, these courses are the only classes teaching this methodology using STELLA," says Hannon. "I have three books coming out, based on what we have learned teaching these courses. One is on the biology aspects of modeling; another is on the economics of natural resources; and a third covers advanced undergraduate engineering, ecology, economics, chemistry, and genetics. Two more will follow on other aspects."

"It was excellent to see the interrelationships in modeling," says Safia Aggarwal, UIUC geography graduate student. Aggarwal will use Hannon's methodology in her thesis on zebra mussels. "The techniques in dealing with the zebra mussel so far have been crude and mostly inadequate. I would like to look at other forms of control, perhaps biological. For example, can a natural predator be prodded into affecting the zebra mussel population?"

Michelle Duffield, English major working towards a degree in Environmental Law, felt the class helped her understand how environmental factors interrelate. "I hope to be able to apply what I have learned in this class to understanding EPA laws that may soon be based on environmental modeling."

An ecological testbed

Hannon and Westervelt had several goals in mind for the Advanced Ecological Modeling class: "While we wanted to show the army the effects of training in the Mojave," says Han-

non, "we mostly wanted to show them the accuracy possible in simulating the ecological processes they are impacting. In addition, we wanted to show students how to model."

"By properly designing the model, we can use it to test ecological theory. In essence, we have created a virtual ecosystem that can also be used as a testbed for ecological theories."

One theory Hannon and Westervelt desire to test involves the mixing of tortoises. "The turtles we are modeling live in clumps scattered across the desert. They get along in their areas for a while, but occasionally they must mix to sustain the genetic makeup."

Hannon says that roads endanger turtles and disturb the mixing process. There are likely no solutions to this problem without bringing harm to the species. "You cannot just run in and take one turtle from Group A to Group B, because you might pick up a diseased one that will kill off the population of Group B. We used this mixing idea in forming our model. We will be able to show turtles in their natural conditions, then add roads and other aspects of human activity to see how each impacts the population level of turtles in the long run."

Establishing the system

A previous Advanced Ecological Modeling class taught by Hannon and Westervelt built a 116,000 cell model of a 20 x 30 mile desert steppe

ecosystem on an army range near Yakima, WA, to study the native Sage Grouse population [see *access*, October–December 1992]. In that simulation, Hannon ran STELLA in a distributed environment using his own Macintosh computer and NCSA's CM-5 system.

The past summer Hannon and Westervelt worked with Thomas Maxwell, University of Maryland at College Park, to convert the STELLA II code to C+ or Fortran for the tortoise model. Hannon and Westervelt then plan to run it on a distributed network of Sun workstations in CERL's laboratory on campus.

The class ended with a complete model of the tortoise and its ecosystem for the generic Mojave cell that was 1 kilometer square together with a full set of initializing GIS "maps" for the fort area. Currently Hannon and Westervelt are transforming the STELLA equations to C+ and arranging the necessary networks of workstations to run the multicellular modeling conglomerate. Their results will be posted on the WWW along with the Sage Grouse model. (See the URL below.)

Planning the next venture

The next step for advanced ecological modeling, regional or global, may be visualization. Hannon and Westervelt created an on-screen "movie" last

Modeling continued on page 27

The Desert Tortoise and Sage Grouse models: <http://ice.gis.uiuc.edu>

As scientific output becomes more complex and high-performance computers crunch enormous datasets, the need to help people make sense of numbers continues.

Scientific visualization is a technique of showing complicated output in an easy-to-understand, data-driven visual representation. Scientists and artists team up to mold a series of 3D pictures of data, such as the graphic representation of a severe storm. In the visualization, weather balloons

change colors and float up or down within clouds to represent changing air flow. Through sonification, sounds could represent air pattern changes.

"Sonification is the next logical follow-on to visualization," says Donna Cox, NCSA's pioneer of the Renaissance Teams approach to scientific visualization. "Sonification is necessary—especially for high-dimensional datasets."

Scientific auditory display

Sounds have the capacity to tell researchers things that cannot be conveyed visually. Scientists are starting to see the benefits sonification gives to their research.

"Sound is complementary to images in everyday life, at the movies, and in computing as well. It reinforces what we see and tells us things we cannot see," says Robin Bargar, a composer of music and research programmer at NCSA. Bargar leads a group of computer scientists, engineers, and composers who are creating ways to enhance virtual environments by adding real-time interactive sound [see *access*, Summer 1994]. Group members include Ulrike Axen (computer science), Sumit Dasa and Kelly Fitz (electrical engineering), Camille Goudeseune (music), and Insook Choi (fine and applied arts).

The Audio Development Group recently produced the NCSA Sound Server, a prototype audio software pipeline used for virtual reality. Bargar says this pipeline does for sonification what SGI's Graphics Pipeline did for visualization. With it, data-driven audio can become an integral component of any software application. "Putting sound and graphics together and showing that sound really made a difference opened the door for the work we are doing today," he says.

He began at NCSA assisting Cox in the production of animations and visualizations, including the well-known *Venus and Milo*, which was featured at SIGGRAPH two years in a row (1990, 1991) in the Computer Graphics and Animation Screening Rooms [see *access*, Sept–Oct 1990; July–August 1991]. Bargar continued producing videos, but his musical background drew him into developing

Data driven sound: The next step

by Victor Ryckaert, Graduate Student, Sangamon State University;
former NCSA Student Intern



A manifold surface for navigating the control space of Chua's circuit. Both input circuit parameter values and output signal are displayed in the same space. This interface was designed by Insook Choi for exploring chaotic systems and generating musical signals. (Courtesy of Bargar and the Audio Development Group)

a way for sound to become a major part of scientific research.

Sound is "one more sensory input in which one can quantify or qualify changes in data," says Cox, UIUC art and design professor and NCSA research scientist. "It acts like our visual perception system in giving us information."

Navigation in the nebulous space of virtual reality is a problem, Cox continues. "It is very difficult to find out where you are in this dataset, or artificial space that is created by the computer," she says. "Using audio to figure out where you are in a space is quite valuable. You can use the changing amplitude of a sound to navigate, like a fish in water."

Pioneering in an "early field"

Establishing the Audio Development Group and creating the server are the latest steps on a journey from music composition to computational science.

Five years ago, auditory display research had little support in the scientific community. Bargar says the vision and imagination of a handful of early supporters like Cox; David Curtis, creative director of NCSA's scientific communications; and Joseph Hardin, associate director of NCSA's Software Development Group, paved the way for today's success. At this early stage, sonification is just beginning to generate acceptance, but it is a long way from the recognition enjoyed by visualization. For example, computing platforms are far behind in providing necessary hardware and software to create high-fidelity audio signals. "Our first research has been to design and build the tools we need to conduct our work," says Bargar. "Now that the server is in place, we can explore methods to create sound patterns that can convey patterns in data, changing over time."

"It's such an early field," says Adrian Freed of Berkeley's Center for New Music and Audio Technology (CNMAT). "There's lots of promise, but the thing that's missing is some very compelling examples of where it works." Examples are beginning to surface, however. Sonification was showcased at SIGGRAPH 94. All 43 VROOM applications included audio provided by the NCSA Sound Server.

To produce data-driven sounds, researchers need a computer that

contains software to manage sound-files and hardware to convert digital data to analog audio signals. It is important to have an audio system attached to the computer that reproduces high-fidelity signals. Since the software to turn data into sound is not standard on most platforms, the Audio Development Group drew on existing computer music software and adapted it to scientific research.

"The computer music community is an untapped resource for computational science and engineering" Bargar says. "Computer musicians—mostly composers—and their engineering collaborators have been inventing hardware and software for producing data-controlled sound for over 30 years."

Forming collaborations

Collaborations are very important for bringing audio into the scientific community. NCSA, through the Audio Development Group, has formed relationships with experts at several prominent centers for computer music and audio signal processing.

The Institute for Research and Coordination of Acoustics and Music (IRCAM) in Paris is one of the original centers for collaborations between computational science and music composition and performance. Xavier Rodet, an audioengineer from IRCAM [see *access*, Spring 1994], assisted Bargar in adapting chaotic circuit equations into a real-time synthesis environment for *Sounds from Chaos in Chua's Circuit* [see *access*, Summer 1994]. One of the world's leading audioengineering researchers in signal processing and physically based models for sound synthesis and musical applications, Rodet has developed important techniques for understanding and creating sounds using spectral representations. These techniques are similar to those used in astrophysics and other sciences.

"Sound is a supplementary information channel that has different properties than the eye. You don't have to face the sound source to hear it; it can wake you up even if you are sleeping," Rodet says. "So by this other channel, more information can be transmitted to a user. This is crucial for very complex information such as highly dimensional structures."

As an example, Rodet points to his study of a version of Chua's circuit called the Time-Delayed Chua's circuit. "The different behaviors—different periods and chaos—are extremely easy to discriminate by ear according to parameter values, whereas this is not so easy by other means."

When asked what sound contributes to science, Rodet replied: "In medicine, the Doppler effect is used to get some information about blood circulation. [The *Doppler effect* is the change in the observed frequency of an acoustic wave caused by the motion of a sound's source and one who observes it.] The corresponding sound is a very convenient way to carry this information to the doctor since he has to look at the measuring device in order to orient it precisely. He could not be looking at a screen at the same time.

"So sonification is a way to help in the exploration of complex data, which appear more and more in modern scientific research. Think of biology or population dynamics, for example."

"These collaborations are important for the transfer of software technology," Bargar adds, "including algorithms and rendering engines, from highly specialized and sometimes inaccessible fields such as computer music and digital sound synthesis, into a much larger scientific user community."

Through another collaboration, Bargar was able to get prototype software to NCSA's server that was developed at CNMAT. The Audio Group adapted the software to NCSA's needs. "We are not working on sonification, but we build tools," says Freed, CNMAT's director of Software and Systems. "Our tools work on SGI machines, and the CAVE is driven by SGI machines. [The NCSA Audio Development Group] took our sound synthesis tools and built layers on top to make them accessible to their audience."

Interactions with science research groups have also been fruitful. In a project involving UIUC's Department of Computer Science and NCSA's Software Development Group, sound is generated by traversing geometric structures called alpha shapes, to

Sound continued on page 16



"It's such an early field," says Adrian Freed, Center for New Music and Audio Technology, University of California, Berkeley.

(Photo by Thompson-McClellan Photography)

Sound continued from page 15

study features that may be hidden in graphical representations [see *access*, Summer 1994]. "Support from Herbert Edelsbrunner [UIUC computer science professor] in terms of ideas and models as well as assistant-

ships for audio personnel really uplifted the Audio Development Group during our formative period," Bargar reported. "We are delighted that one of Herbert's students is now a regular member of the Audio Development Group and is considering sound as part of her doctoral thesis."

Ongoing interactions between the CCSR (Center for Complex Systems Research) and the Audio Development Group have led to a number of exciting projects involving the sonification and visualization of nonlinear dynamical systems and "deterministic chaos." In particular, these interactions formed the basis for the use of the chaotic behavior of the Chua circuit in musical composition [see *access*, Summer 1994], provided an important test case for development of the CAVE interface, and are currently suggesting more effective and appealing ways of rendering sound from EEG patterns and of producing acoustic stimuli for inducing EEG responses in laboratory tests.

"We look forward in the near future," adds Bargar, "to establishing a dedicated audio facility where researchers can collaborate with NCSA to produce sound from their computational models."

Sonification for industry

Bargar's audience ranges beyond research scientists to NCSA's industrial partners. For example, Caterpillar Inc. researchers are starting to see the payoff sonification can bring to industry.

"We hope that by adding sound to our virtual reality CAVE environment, we can create a more realistic virtual prototype of our vehicles," says Kem Ahlers, manager of University Relations for Caterpillar on-site at NCSA. "By making a more realistic virtual prototype of Caterpillar tractors, we can reduce the amount of costly iron prototypes we must build, and we are able to evaluate many more potential designs. This creates a product that has more value to our customers and means more profit. We can also bring those designs to market quicker, which we need to do to compete in this new global marketplace. All of these hopefully translate into more profit for Caterpillar."

Expanding sound technology

With the advancement of technology into contemporary culture, Bargar notes that the scope of sonification can reach beyond the CAVE.

"Sonification is one corner of the field of auditory display that is becoming increasingly important for many segments of the computer community," he says. "In the past, computers were only accessible by numerals and by text. More recently, graphics revolutionized the ability of the computer and user to interact. With multimedia computing upon us, computers are being built to reproduce sound with the same quality as a home compact-disc player and stereo system. This means that audio tools and computed sounds now have more ways to be heard than ever before."

"Sound—produced and controlled by computed data—will play a larger role in these environments as people learn how to approach sound from a computational perspective and as tools become established in the form of stable software."

For further readings, see the WWW online version of this article in *access* using NCSA Mosaic.

NOTE: For examples of these applications, look for the NCSA Audio Development Group's WWW Home Page later this fall. ▲

Jupiter countdown by Larry Smarr, Director of NCSA

On Monday, July 17, 1994 Larry Smarr wrote the NCSA Staff:

"So far Fragments A, B, & C of the Shoemaker-Levy 9 comet hitting Jupiter have hit. There are pictures that capture the fireball (Calar Alto Observatory in Spain) emerging above the limb of Jupiter just after the impact, close ups of the "wound" left in Jupiter's atmosphere by Fragment A (from the Hubble Space Telescope), a nice sequence of the impact sites of Fragment A and C (from the Anglo Australian Telescope), and a stunning close up of the impact sites of A and C by the largest Earth-based telescope (from Keck Observatory). Apparently Fragment B was a 'dud'. The remaining fragments will rain in all during the week. Follow the action on NCSA Mosaic!

"The first impact confirms the predictions made by a detailed supercomputer simulation of the impact carried out by long-time NCSA Researcher Mordecai-Mark Mac Low and his colleagues using the ZEUS code developed in NCSA Research Scientist Michael Norman's NCSA Astrophysics Group and run on the CRAY C-90 system at PSC [see *access*, Summer 1994]. A similar computation was carried out at Sandia National Laboratories on the large Paragon which was obtained thru the NCHPC (National Consortium for High Performance Computing).

This is Grand Challenge style science using the NSF MetaCenter or National Consortium. It is a harbinger of changes in science leading to a worldwide networked collaborative effort. We will see more of such in the 1990s. Notice how intertwined components of HPCC (supercomputers, application code development, multiple centers) and NII (NCSA Mosaic/WWW, remote instruments networked together, global interactive collaboration) are involved in this piece of science!

The URL for the images taken worldwide plus in space is
<http://newproducts.jpl.nasa.gov/sl9/sl9.html>

NCSA sponsors

SuperQuest

FOR TEACHERS

by Sara Latta, Science Writer

For three weeks this past summer, 24 high school teachers of science and mathematics became students again at NCSA's SuperQuest for Teachers workshop. They learned how to run, modify, and write computer models, and how to use visualization to bring their models to life. (Participants are listed in the sidebar on page 19.)

The teachers, in teams of two or three, came from small rural schools with only a few computers, as well as large, technology-rich schools. One team of teachers developed a model that describes the behavior of model rockets for a physics class; a biology-physics teacher team chose to model the physics of animal movement for use in their respective classes. In short, the teachers learned how to use computational science in the classroom.

One team, **John Biggerstaff** and **Jim Nazworthy**, teach mathematics—calculus and physics respectively at a large suburban high school in Lee's Summit, MO. The school, which is no stranger to computers and access to the Internet, is offering a new course in computational science taught by Biggerstaff and Nazworthy. "We wanted to come up with some ideas and starting points for [the course's section on modeling and simulation]," says Biggerstaff. "This course will give students the opportunity to create their own learning—to move away from the teacher as simply a dispenser of knowledge. For us,

it's not just modeling for the sake of modeling, but a vehicle for taking education the way we think it ought to go."

Using online resources

For some teachers, SuperQuest provided the opportunity to access educational resources via the Internet. "I wanted to come to this workshop because I think the Internet has great capability of reaching small schools that are isolated," said **Elwood Gruschow**, who teaches chemistry, physical science, physics, pre-algebra, tech-prep math, and computer literacy in a small rural high school in Sidell, IL. "I came for the connectivity part of this workshop as much as anything."

Gruschow and teammate **Linda Rosnett** (who teaches a computer programming class) want to show their students how computers could be used to model everyday activities. "In previous classes, we have had to use frictionless surfaces and ideal objects [to learn about physical laws], but we can do real-world stuff with a computer," concludes Gruschow.

Honing computational skills

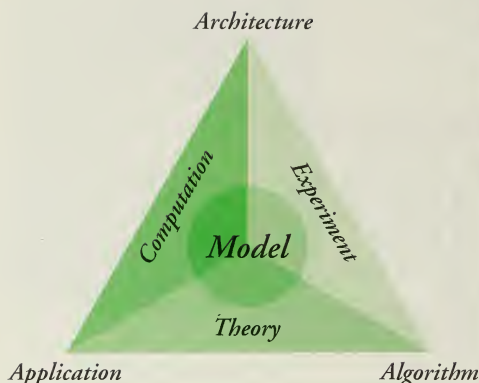
The teachers attended lectures and labs to learn about modeling, computational science, and computer skills led by a team of two university faculty, an education researcher, a high school teacher, four graduate students, and five undergraduate interns. In lab sessions, they learned

how to use software tools that would help them in their classroom: STELLA II, *Mathematica*, Interactive Physics, ChemViz, TrueBASIC, and Excel. They honed their newly learned skills by working in groups to develop new computer models.

A recurring example used in lectures on modeling was the growth of rabbit populations, which led one team to model an imaginary illness called SuperQuestitis. The main "symptom" of the illness is having hallucinations about many, many rabbits. (The model actually showed how bacteria can acquire resistance to antibiotics after several generations.) At the end of the workshop, the original teacher-teams gave presentations summarizing their work and the ways in which they hoped to use computational science in their classrooms.

The workshop, which was sponsored by NCSA's Education Group and funded by NSF, replaced the previous years' SuperQuest programs [see *access*, July–August 1991; July–September 1992; and Spring and Fall 1993] that targeted teams of high school students along with teacher-coaches. NCSA, together with other SuperQuest centers and NSF, concluded that their efforts to bring computational science to the classroom would be multiplied by having a teacher-centered, rather than student-centered, program.

SuperQuest continued on page 18



SuperQuest '94 logo designed by Bob Panoff and Ben Davenport. (Courtesy of NCSA Education Outreach Group)
Michael South (left) helps Melissa Steffens, SuperQuest '94 attendee from Missouri. (Photo by Thompson-McClellan Photography)



SuperQuest continued from page 17

Expanding horizons

The workshop expanded the horizons of people who work with teachers as well. Two of NCSA's educational affiliates, TENET (statewide educational network in Texas) and ShareNet (educational network in the Kansas City area) sent representatives who took part in the workshop and learned about methods of teaching computational science to teachers. **Coco Conn**, producer of a VROOM project called *CitySpace* that helps young people design cities of the future and look at them using virtual reality [see *access*, Summer 1994], came to observe and learn more about teachers' needs.

Teachers from the Ramstein American High School, Ramstein, Germany, also attended under the auspices of the U.S. Department of Defense Dependent Services.

Year-long support

SuperQuest for Teachers did not end with the three-week workshop. NCSA's Education Group provides follow-up support in Chris Kolar, graduate student in the College of Education. Kolar answers any questions the teachers may have from "How do I get this package to work

on my machine?" or "Do you have any ideas on modeling this mathematical concept?"

NCSA has also set up an electronic mail reflector that the teachers use extensively to send news of what is new in the classroom, to ask other teachers questions, or to stay in touch. Either Bob Panoff, NCSA visiting scientist in the Education Group and coordinator of SuperQuest for Teachers; Kolar; or both will conduct an on-site visit to each participating school during the fall or spring semester. "We will meet with other teachers, the principal, or administrators—even the PTA or school board—to explain the program," says Panoff. "We will hold a workshop for other teachers if that's what they want, assess their equipment situation, and make further recommendations."

In addition, the teachers will receive items from their "wish list": in most cases, software packages like the ones used in the workshop. An exception might be money to help defray the cost of a long-distance

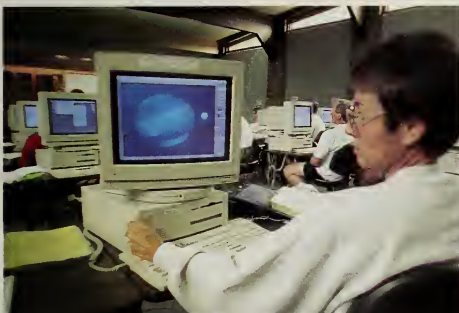
telephone hookup to the Internet for some of the rural schools, for example.

During SuperQuest, a newspaper called the *Daily Observer* was published every day using NCSA Mosaic. Throughout the next school year, the newspaper and other pertinent information related to SuperQuest and the Education Group's program will be available online at the URL given below.

Gruschow: "I would attend [again]"

The worth of the workshop was perhaps best summarized by Gruschow, who sent this message to Panoff afterwards: "My family and I just returned from Utah [on vacation]. Now I have until the 23rd [of August] to finish the bathroom remodeling I quit working on to attend SuperQuest for Teachers. If I again had the choice to attend SuperQuest for Teachers or have an acceptable bathroom in our one-bathroom house, I would attend SuperQuest for Teachers." ▲

SuperQuest and other education information is available at:
<http://www.ncsa.uiuc.edu/edu/superquest/sqt>



Above: Wallace Fegert and Susan Bahe (left and right front row), teachers from North Dakota, listen attentively.

Below: Judy Word, teacher from Missouri, gets hands-on experience at SuperQuest '94. (Photos by Thompson-McClellan Photography)

SuperQuest '94 attendees

Wallace Fegert, Lakota Public Schools, Lakota, ND
 Susan Bahe, Lakota Public Schools, Lakota, ND
 Kent Brown, Upham Public Schools, Upham, ND
 Harlan Heinrich, Upham Public Schools, Upham, ND
 Al Fleming, Centennial HS, Champaign, IL
 Elizabeth Sudlow, Centennial HS, Champaign, IL
 Elwood Gruschow, Jamaica HS, Sidell, IL
 Linda Rosnett, Jamaica HS, Sidell, IL
 John Biggerstaff, Lee's Summit HS, Lee's Summit, MO
 Jim Nazworthy, Lee's Summit HS, Lee's Summit, MO
 David Brunsting, Emmerich Manual HS, Indianapolis, IN
 Don Gilroy, Greenfield Central HS, Greenfield, IN
 Robert Flegel, Bird Island-Olivia Lake Lillian District Sr. High School, (BOLD HS), Olivia, MN
 Robert Remsberg, BOLD HS, Olivia, MN
 Brad Goral, New Trier HS, Winnetka, IL
 Terry Sullivan, Oakland HS, Oakland, IL
 Ellen Massey, Oak Grove R-6 Schools, Oak Grove, MO
 Jill Vinke, Oak Grove R-6 Schools, Oak Grove, MO
 Judy Word, Oak Grove R-6 Schools, Oak Grove, MO
 Debra Brueck, Truman HS, Independence, MO
 Melissa Steffens, Truman HS, Independence, MO
 *Coco Conn, Internet Tours, Hollywood, CA
 *Rick Kartchner, (DoDDS) Ramstein American HS, Germany
 *Edward Milner, (DoDDS) Ramstein American HS, Germany
 *Terri Nguyen, DoD Education Activity, DoD
 Lane Scott, TENET/TX Educ. Agency, Austin, TX
 Nelson Thomas, TENET/Blocker Middle School, Texas City, TX
 Christy Wessinger, Sharenet/PEI, Kansas City, MO

*Not in teams and not NSF funded (see text)

See page 23 for information on how NCSA's Education Group brought the Illinois State Fair online.

1994 Undergraduate Computational Science Award for GalaxSee

Two interactive simulations **Bob Panoff** developed with students this past year, SimSurface and GalaxSee [see *access*, Spring 1994], along with another computational science problem Panoff submitted with colleagues at Clemson University were combined and awarded one of thirteen 1994 Undergraduate Computational Science Awards.

The recognition program is an initiative of the U.S. Department of Energy and is administered by NASA Ames Laboratory. **Amy Biermann** (1994 REU Student from Bryn Mawr College) and **Ben Davenport** (1993 and 1994 Summer Intern from Princeton University) were

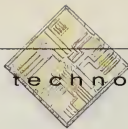
co-authors with Panoff. Their work is part of a larger effort at NCSA to develop a set of scientific simulations for classroom use.

In addition to the recognition and a certificate, a cash award of \$1,000 went to the authors. Travel funds to attend an award ceremony and poster session held in Washington, DC in September was part of the award as well.

Earlier in the year, GalaxSee and Panoff had received recognition from the Office of the Director of Defense Research and Engineering, via Capt. Bruce McClure, director of Defense Modeling and Simulation Office of the U.S. Navy.

In a letter of commendation to Panoff, McClure commented: "Access to the computing power of the university's Cray supercomputer through the Internet allowed students a unique opportunity to study the origin of the universe [using GalaxSee] which would be impossible with computers on campus at high schools."

Panoff introduced distributed, interactive learning demonstrations, including GalaxSee, to attendees at the 15th Annual Interservice/Industry Training Systems and Education Conference. ▲



HTML for World Wide Web users

by Ginny Hudak-David, Publications Editor, Publications Group

Illustrations by John Havlik

"Is this HTML coding stuff really hard to do? How do I get started creating a file for a World Wide Web server?"

Jennie File, NCSA's Software Development Group trainer, reports being asked these and similar questions a lot during her training sessions for a variety of audiences, including NCSA staff. "Many people seem to think that they won't be able to do this—but they find out they can!"

Using HTML is not as difficult as you might think, and using NCSA Mosaic to view your efforts is particularly rewarding because of its graphics display capabilities.

NCSA Mosaic and the WWW

NCSA Mosaic software [see *access*, Fall 1993] is a browser—a hypermedia network navigation tool that lets you access information on the Internet by clicking on hyperlinks, also called anchors, in formatted documents. NCSA Mosaic formats files provided on *servers*, or computers that offer services and files to other machines. NCSA Mosaic is available for the Macintosh, X Window System, and Microsoft Windows platforms.

World Wide Web (WWW) servers use the HyperText Transfer Protocol (HTTP) to provide files. (Files can also be read from Gopher and anonymous FTP servers.) Files are identified by Uniform Resource Locators (URLs), which can be considered a file's address. A URL combines the server protocol, usually HTTP, with the machine address, the file's directory, and the filename in the following format:

protocol://machineaddress/directory/filename

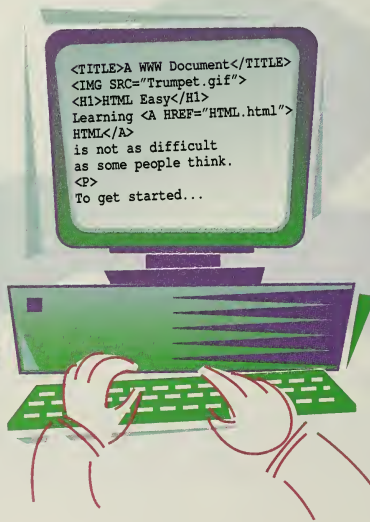
HTML

Text files are coded for display in NCSA Mosaic (or in other Web browsers) using the Web formatting language called HTML (HyperText Markup Language), which is a subset of the Standard Generalized Markup Language (SGML). All word-processing software uses some kind of markup language, but the software you use probably hides the codes that tell your monitor or printer to show a word in boldface type, for example. When you create an HTML file, you insert a code or *tag* that tells the browser how to display some text, but the tag is visible only in the original file (see the illustrations). If you have never used a markup language, this may be a different way of thinking about a file. If you have used TeX or LaTeX, moving to HTML is easy.

One thing about browsers and coded files is a change for many authors—you are not able to have complete control over the final presentation of information. For example, in a word-processed document you can format a heading as you like: bold, larger point size, different font, centered. You design the page layout to suit the needs of your readers and to integrate with other documents as necessary. In an HTML-coded file, however, you tag the specific elements of the file, but the browser software formats the final presentation. This means that you cannot specify many details of the final presentation.

Getting started

Start by creating an ASCII text file—that is, either change an existing word-processed document into a text file by saving it as text with line breaks or start a new file as a text file. Common UNIX text processors are vi and EMACS; Macintosh users can try BBEdit, or their favorite word processor with carriage returns inserted at the



end of each line prior to the final file save. Name your file with the .html extension (e.g., xfile.html).

Pairs of tags enclosed in angle brackets (< >) instruct the browser to format headings, insert graphics, or display words in bold or italics. The first angle-bracket tag starts the instruction; the second code angle-bracket tag—with the addition of a leading slash mark (</>)—ends the tag's instructions. If you are marking a first-level heading in your file, enclose the text between the level one heading tags as shown: <h1>Hardware enhancements</h1>. There are HTML tags for lists, quotations, headings, emphasis, and other common presentation styles. (See "For more information" below.)

Hyperlinks

Hyperlinks connect words or graphics with related files located anywhere on the Internet. WWW browsers display the hyperlink anchor in color or underlined. Hyperlinks can point to text, image, sound, or movie files.

To include a hyperlink in a file, you must have the file's URL. For example, to make a hyperlink to the NCSA Home Page, you would include this HTML code:

```
<a href="http://www.ncsa.uiuc.edu/General/
NCSAHome.html">NCSA</a>
```

The href= section gives the file's URL enclosed within quotation marks. The word NCSA, enclosed between the right angle bracket (>) and the end of the anchor tag (), will be shown in color or underlined in your window. (The start of the anchor tag is at the very beginning: <a.)

Graphics

Most file authors want to include graphics in their files. NCSA Mosaic can display X bitmap or GIF file format images inside a formatted document. Graphics are scanned and manipulated using an art production tool such as Adobe Photoshop.

Scan, size, and save your image in an X bitmap or GIF format. Use the appropriate extension when naming your file (.xbm, .gif). You can also create and save images from your monitor screen by using a program such as FlashIt for the Macintosh, a screen-capture utility that freezes your screen and lets you take a snapshot of any or all of the current display.

To include a graphic in your file, use the tag, which tells your browser to retrieve and display the image file referenced in the URL. In this example, the file that will be displayed shows the copyright symbol (©):

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Putting it together

Once you have your HTML coded file and any graphics files created, you may want to make them available to the Internet community. Sharing information requires a WWW, Gopher, or anonymous FTP server. For information on establishing a WWW server, see "For more information" below.

By putting the pieces together—HTML tags, images, and hyperlinks—you can create an interesting and informative formatted document that tells other Internet surfers about your work. Maybe you will be able to say, as someone recently did to Jennie File, "Gee, this is fun!"

For more information

Refer to the following online files for additional information:

A Beginner's Guide to HTML

<http://www.ncsa.uiuc.edu/General/Internet/WWW/HTMLPrimer.html>

A Beginner's Guide to URLs

<http://www.ncsa.uiuc.edu/demoweb/url-primer.html>

Information about HTML

<http://info.cern.ch/hypertext/WWW/MarkUp/MarkUp.html>

Establishing a server

<http://hoohoo.ncsa.uiuc.edu/docs/Overview.html>

More information on NCSA Mosaic

<http://www.ncsa.uiuc.edu/SDG/Software/Mosaic/NCSAMosaicHome.html> ▲



NCSA MOSAIC LICENSING

To better meet the strong market demand for easy-to-use Internet access tools, Spyglass Inc. and the UIUC announced in August a master-license agreement that assigned to Spyglass all future commercial licensing rights for NCSA Mosaic.

Spyglass, an NCSA spin-off company founded in 1990, develops visual data analysis software tools for engineers and scientists. Under this agreement, it distributes commercially enhanced versions of NCSA Mosaic for Windows, Macintosh, and UNIX platforms. Spyglass licenses its Enhanced NCSA Mosaic to networking software companies, systems vendors, and online service providers for incorporation into their products and services.

NCSA Mosaic gives users point-and-click access to the World Wide Web (WWW) [see *access*, Fall 1993]. More than two million copies of NCSA Mosaic are in use, and an additional 60,000 copies are downloaded each month from the NCSA anonymous FTP server.

The UIUC-Spyglass agreement creates a broader, more practical distribution channel for commercial versions of NCSA Mosaic. NCSA Mosaic has been available free with copyright to individuals or through a limited number of commercial licensees [see *access*, Spring 1994].

"With the overwhelming demand for commercial versions of Mosaic, our distribution system needed to be dramatically strengthened," said NCSA Director Larry Smarr last August. "Working with Spyglass, we can get NCSA Mosaic to everyone who wants it much more quickly—largely by mobilizing lots of vendors who will integrate, add value to, and incorporate Enhanced NCSA Mosaic with their products for distribution to their customers. We believe that this arrangement will free up NCSA developers to work on adding new leading-edge capabilities to NCSA Mosaic."

"This new agreement solves the problem of getting solid, commercial-quality copies of NCSA Mosaic to the tens of millions of people who want to tap the rich resources of the World Wide Web and the Internet," said

Douglas Colbeth, Spyglass's president. "It will give vendors stable, standard, and feature-rich versions of Enhanced NCSA Mosaic that they can incorporate immediately into their products—with little or no additional development work, if they so choose."

"Our ultimate goal is to have people automatically receive Enhanced NCSA Mosaic as a standard part of their computer systems, networking software, and commercial online services. By this time next year, there should be more than 20 million copies of Enhanced NCSA Mosaic from Spyglass in use on desktops."

UIUC is honoring all agreements with current commercial licensees, but is referring inquiries about future commercial licenses to Spyglass and encouraging current licensees to work with Spyglass. Because Spyglass has committed to license very high volumes of NCSA Mosaic licenses from UIUC, the company can offer Enhanced NCSA Mosaic to licensees at favorable terms.

This UIUC-Spyglass agreement is an extension of a multimillion-dollar joint development and licensing agreement signed in May 1994. Under the agreement, NCSA now focuses on research into advanced features for the next generations of NCSA Mosaic—such as voice recognition, full-motion video, and intelligent agents for searching the Internet. Spyglass is developing and bringing to market commercially enhanced versions of NCSA Mosaic, focusing on large-volume sales to other vendors.

NCSA continues to offer a public-with-copyright version of NCSA Mosaic via the Internet that can be downloaded free. As part of its agreement with NCSA, Spyglass is providing a number of its improvements to NCSA for incorporation into NCSA's public-with-copyright version.

For more information, contact Spyglass Inc. at (217) 355-6000 or the URL below.

NCSA Mosaic licensing:
<http://www.spyglass.com>

SPYGLASS LICENSING PARTNERS

In August 1994, Spyglass Inc. announced the formation of relationships with IBM's Networking Software Division, Research Triangle Park, NC; FTP Software Inc., North Andover, MA; O'Reilly and Associates Inc., Sebastopol, CA; and Firefox Inc., San Jose, CA. Since becoming a commercial licensee of NCSA Mosaic, Spyglass has licensed more than 5 million copies of its Enhanced NCSA Mosaic to these companies and others that are integrating it into their products.

IBM's family of TCP/IP products provides a comprehensive set of applications to meet the interoperability and connectivity needs of business and home users. By integrating Enhanced NCSA Mosaic from Spyglass with IBM's TCP/IP application suite, IBM provides users with leading graphical facilities for accessing and navigating the Internet.

FTP Software, a popular producer of TCP/IP internetworking software, develops products that combine workgroup TCP/IP software with high-end features of enterprise environments. FTP Software plans to incorporate NCSA Mosaic technology into its future products.

O'Reilly and Associates is a popular publisher of books about the Internet, including *The Whole Internet User's Guide and Catalog* [see *access*, Fall 1993] and developer of Global Network Navigator (GNN) that links more than 650 Internet information servers. O'Reilly has licensed Enhanced NCSA Mosaic from Spyglass and will bundle the software with *The Mosaic Handbook* to be published in three editions (for Windows, Macintosh, and X Window System platforms).

The book is scheduled to be in bookstores this fall. O'Reilly's Digital Media Group (DMG) will distribute Enhanced NCSA Mosaic to GNN users who want a commercially supported version of NCSA Mosaic. DMG will license NCSA Mosaic to other digital Internet-based publishers.

Firefox Corporation Ltd., a popular provider of server-based TCP/IP communications services for use in Novell's NetWare environments, plans to provide Enhanced NCSA

Mosaic as an integral part of its expanded NOVIX product line. NOVIX enhances NetWare by centralizing the administration, management, and security of TCP/IP communications and access at the NetWare server. Firefox's products are available through Novell.

STATE FAIR ONLINE

The Illinois State Fair is the first state fair to have information on the WWW on an Internet connection. The 1994 Illinois State Fair marked the 175th anniversary of Illinois statehood.

In collaboration with Illinois Lieutenant Governor Bob Kustra's office, Ameritech, UIUC's Computing and Communications Services Office, and the Illinois Math and Science Academy, NCSA's Education Group worked to bring the daily schedule and reports of many special events to the WWW community.

More than 43,000 users accessed this display during the last two weeks of August alone. NCSA Visiting Scientist Bob Panoff, who was responsible for getting the information online on NCSA's WWW server, reported receiving many electronic mail messages from displaced Illinoisians who lamented not being able to make it back for the fair. Said Pat Ridge, a high school teacher at an American school in Germany, "The Home Page for the Illinois State Fair looks great! How do I purchase my cotton candy?"

The state fair exhibit is still available, so you can bring back a bit of the summer by visiting it via the URL below.

Look for information about the state's efforts to coordinate resources and services to promote increased use of computers and other new technologies for Illinois classrooms in a future issue of *access*.

Illinois State Fair:
<http://www.ncsa.uiuc.edu/edu/StateFair/FairHome.html>



Used with permission from *SCIENCE*, vol. 265, cover, Aug. 12, 1994.

NCSA MOSAIC FEATURED IN *SCIENCE*

The past, present, and future technology of network information systems on the Internet, focusing on WWW and NCSA Mosaic, was the cover article in the August 12, 1994, issue of *Science* that featured computing.

Bruce Schatz, NCSA research scientist, and Joseph Hardin, associate director of NCSA's Software Development Group, co-authored the article entitled "NCSA Mosaic and the World Wide Web: Global Hypermedia Protocols for the Internet." It was the first article (text, figures, and cover) submitted to *Science* electronically.

Ingrid Kallick, graphic designer in NCSA's Publications Group, designed the cover of *Science*, which was a montage of NCSA Mosaic screen images capturing displays on WWW servers around the world. The following blurb described the cover illustration:

"Composite of computer screens above a globe roughly corresponding to the location of the data. The screens were created with Mosaic software developed at the National Center for Supercomputing Applications (NCSA) for browsing the World Wide Web. This Internet technology enables scientists to make their information rapidly available to the global community. These and other issues are discussed in this special issue on computing. See the Editorial on page 851 and News Reports, Perspectives, and Articles beginning on page 879. [Image: I. Kallick and B. Schatz at NCSA, using public domain sources on the Internet]"

Images used were from WWW exhibits of the following organizations: CERN, JPL, NIH, UC Berkeley, UIUC, and NCSA.

Science is published weekly, except the last week of December, by the American Association for the Advancement of Science.

NCSA TRANSFERS TECHNOLOGY TO THE SILICON PRAIRIE BY ALAINA KANFER, NCSA EDUCATION OUTREACH

Champaign County Network (CCNet) has moved out of the planning stages and into sites around the county. Centerwide efforts have provided technical, educational, and organizational contributions to CCNet, which is spearheaded by the Champaign County Chamber of Commerce [see *access*, Spring 1993; Spring 1994].

Now anyone in Champaign County can explore the Internet using NCSA Mosaic via a high-speed CCNet connection.

Connections

Eight schools in Champaign-Urbana have ISDN (Integrated Services Digital Network) connections to the Internet through a joint project with Ameritech and UIUC's Computing and Communications Services Office. Three high schools in the cities are being connected to Internet with remote link adapters (RLAs), an asymmetric networking solution from Hybrid Technologies Inc. in California.

The RLAs enable high-speed transmission through a cable channel provided for this pilot project by Time-Warner/Cablevision. Out-going data transmission is at modem speed over a telephone line. The Hybrid equipment provides sufficient bandwidth to readily access information from the WWW via NCSA Mosaic. Currently being tested are technologies with very high transmission rates, including wireless technologies,

that allow for providing as well as accessing large amounts of information.

The Urbana Free Library is Champaign County's first public CCNet site. Library patrons can discover and retrieve information using a personal computer fully equipped with sound, image, and video viewers connected to the Internet via a Hybrid RLA.

Champaign County businesses are able to conduct their business via Internet. As the first business site of CCNet, Monarch Color Company of Champaign can receive files to print from their local clients connected to the Internet. Other businesses were scheduled to be connected this fall prior to press time.

While CCNet offers high-speed information access and communication, Prairienet, the local FreeNet, offers free modem connections to the Internet and provides local information in text-only and HTML formats. Prairienet, operated largely by volunteers, is managed by UIUC's Graduate School of Library and Information Science.

Online exhibits

The Silicon Prairie exhibit provides a glimpse of Champaign County to Internet users around the world, with general descriptions and images of communities within Champaign County. The



Press conference for the installation of CCNet's Hybrid RLA at the Urbana Free Library was attended by a diverse community group. NCSA Director Larry Smarr participated in the presentation. (Photo by Thompson-McClellan Photography)

exhibit also provides information about National Information Infrastructure activities in the county, as well as listings and directories of interest to the local community. See the URL below.

Several local businesses are in the process of creating HTML documents for their own exhibits on the WWW using NCSA Mosaic software.

Continued outreach

To date, more than 200 individuals and over 70 organizations around the county have contributed to CCNet efforts. While CCNet is developing quickly and the involvement of people continues to grow, CCNet members realize the importance

of keeping Champaign County's leaders updated.

A September presentation was given to county leaders, including Champaign and Urbana city councils, Champaign County board, Chamber of Commerce board, Champaign-Urbana Community Visitors' Bureau board members, and school board presidents.

It showcased a CCNet video, Champaign County NCSA Mosaic exhibits, examples of the benefits of electronic communications, and applications of Geographic Information Systems [see *access*, Spring 1994], both inside and outside the county. ▲

Champaign County's Silicon Prairie exhibit:
<http://www.prairienet.org/SiliconPrairie/ccnet.html>

MILESTONES

New staff

John Ziebarth, NCSA's new associate director for Education and Outreach, comes to NCSA from the computer science department of the University of Alabama, Huntsville, where he was also director of education for the Alabama Supercomputing Center.

While at the center, he developed the Alabama Precollege Supercomputing Program for high school students to learn about computational science and supercomputing. Developed by NASA, the statewide program involves students and teachers from about 100 high schools. Like NCSA, the Alabama Supercomputing Center is a site of the NSF-sponsored SuperQuest Program.

John Melchi became NCSA's Public Information Officer in August. Now in NCSA's Director's Office, Melchi was formerly publications manager for Alpha Tau Omega Fraternity National Headquarters located in Champaign.

In the early nineties, he was a public information intern and later a freelance science writer/photographer for NCSA. Melchi is filling the position of Jarrett Cohen, who went to Hughes STX Corp. last spring [see *access*, Spring 1994].

Student intern **Christopher Adasiewicz** is assigned to the Director's Office and the Publications Group. He joined NCSA this fall to fill the position of Victor Ryckaert, now in graduate school at Sangamon State University, Springfield, IL.

Holly Korab recently joined NCSA's Publications Group as a science and technical writer of online hypermedia presentations and other documentation and outreach projects. Before coming to NCSA, Korab was a research information specialist at UIUC's Institute for Environmental Studies.

Staff changes

David Curtis recently stepped aside as associate director for Scientific Communications and Media Services (SCMS) to lead a centerwide team that focuses on development of programmatic content for video-intensive, online hypermedia for education and outreach.

Tony Baylis, formerly of SCMS, is team leader of Media Technology Resources, which has been integrated into User Services.

Vincent Jurgens, former team leader of Media Services, is now a team leader in the Virtual Environments Group (VEG).

Eric Katz moved into the Publications Group to work on NCSA Mosaic outreach and information support. Formerly with Computing and Communications (C&C), Katz worked on AFS during its introduction and became NCSA's WWW server administrator. He stepped into the vacancy left by **Kenneth Chang**, who was accepted into the science writing program at the University of California, Santa Cruz.

Chris Zollars is Project Manager for Supercomputing '94, coordinating the National MetaCenter exhibit in Cohen's absence. Formerly with SCMS, Zollars just completed a master's degree in Journalism at UIUC.



"A Worker House-Home" is the title of a short documentary made by local students that aired on Champaign-Urbana's PBS station. University High School English teacher Audrey Wells (foreground) thought some of the students in her class on social advocacy might discover the impact of TV on their lives by producing a documentary about a volunteer project. NCSA Video Producer Jay Rosenstein (center right in dark shirt) trained students on the equipment, facilitated the scripting, and edited the video. Production equipment was loaned by NCSA and WILL-TV (UIUC-sponsored PBS affiliate). NCSA provided all the postproduction equipment. Others who took part in a presentation and viewing of the documentary in NCSA's editing suite were (left to right) Elizabeth Murphy (student), University High School Principal Shelley Roberts, Cathy Goodall, and Jordan Finkin (students). (Photo by Thompson-McClellan Photography)

Milestones continued on page 26



David Ceperley (Photo by Thompson-McClellan Photography)

David Ceperley, research scientist with NCSA's Applications Group, won the fifth Eugene Feenberg Memorial Medal for his contributions to computational many-body physics. His work has opened a new era of understanding strongly interacting quantum systems and paved the way to quantitative microscopic prediction of the properties of real, complex materials.

Among Ceperley's celebrated work are calculations he performed, with Richard Martin and Vinnie Natolie, on NCSA's CRAY Y/MP system to establish the series of crystalline phase transitions hydrogen undergoes as it is compressed to several million atmospheres of pressure, a condition present in the interiors of giant planets.

"The award indicates how much of an impact computational physics is making on a very important field of physics, the theory of quantum systems," Ceperley says. Ceperley, who joined NCSA in 1987, is 44. The distinguished award comes at the middle of his career.

The Feenberg medal is presented every two to three years at the Conference on Recent Progress in Many Body Theories. It was first awarded in 1985, and it is named in honor of Eugene Feenberg to commemorate his accomplishments and contributions to physics. Past recipients are David Pines (1985), John W. Clark (1987), Malvin H. Kalos (1989), and Walter Kohn (1991).

Feenberg held the Wayman Crow Professorship at Washington University, St. Louis, in the 1970s. He hoped science would be able to transcend model problems and make quantitatively accurate predictions of the properties of strongly interacting quantum systems under realistic conditions. Ceperley has done just that for a wide range of quantum many-body systems.

Ceperley's most notable contribution has been the calculation, with Berni Alder, of the energy of an electron liquid. The computation is arguably valuable; it provides basic input data for virtually every current numerical application of density functional theory to electronic systems.

Ceperley is a full professor of physics at UIUC. He has a bachelor's in physics and mathematics from the University of Michigan and a doctorate in physics from Cornell University, where Kalos was his mentor. ▲

Moving on

Curt Canada has relocated to Los Alamos National Laboratory (LANL) in New Mexico. As a long-time NCSA research programmer, Canada led efforts in mass storage and database tools and most recently managed NCSA's CM-5. He is in the Advanced Computing Laboratory at LANL where he will be working on the CM-5 and other systems.

Daniel Weber recently left NCSA to focus on graduate studies at UIUC. Weber, who was an on-site resource for scientists and other users at the Beckman Institute, worked on the BLANCA Testbed project when first at NCSA.

Lisa Bievenue recently left NCSA to teach multimedia, hypermedia, desktop publishing, and mathematics or physics at Centennial High School, Champaign. She continues to work on NCSA education projects.

Awards

Orville Vernon Burton, UIUC history professor, is one of 31 national fellows appointed to the National Humanities Center in Washington, DC, for the current academic year. Burton's research covers many aspects of the American South [see *access*, October–December 1992]. This grant will enable him to research localism and nationalism during the Confederacy.

access placed second in the newsletter category in the In-Plant Management Association's annual publication/printing competition for 1993-94. ▲



Scott Mutter, renowned Chicago photomontage artist who for over 20 years has worked exclusively in the darkroom, touched a computer for the first time last spring at the UIUC's Beckman Institute's Visualization Facility. As a visiting artist, he was able to use the center's visualization facility at the in-house rate of \$20 a month and had the technical support of lab monitors, such as Kate Llewelyn.

Donna Cox, member of NCSA's Virtual Environments Group and UIUC professor of art/design, was instrumental in bringing the artist to the Beckman Institute. (Photo and caption by Victor Ryckaert, graduate student at Sangamon State University)



VROOM (virtual reality room) was a popular exhibit at SIGGRAPH 94 [see access, Summer 1994] if these lines of attendees waiting to get in are evidence. (Photo by Lynn Gephart, NCSA Media Technology Resources)

Modeling continued from page 13

year to show the life-cycle of the Sage Grouse. While the movie is not quantitative, it is an excellent low-resolution way to show qualitative information about how grouse mating patterns are disturbed by the noise of army maneuvers. Visualization is thought to be more effective in delivering a message about population changes than charts or graphs.

The Desert Tortoise model will predict increasing vehicular effects on green vegetative cover due to soil compaction. Vegetation could shift from shrubs to annuals, meaning less food for the tortoise. In addition, there may already be observable impact from the army's training exercises. The Desert Tortoise now congregates in certain areas of the range, rather than the more random widespread distribution expected.

Hannon and Westervelt are well on their way to helping the army understand how its use of the Mojave Desert impacts the Desert Tortoise. Perhaps more importantly, they are helping students understand many interrelated factors that control and affect their environment. ▲

CRAY Y-MP continued from page 11

Verifying this theory is difficult, however. A reasonably complete model of the atmosphere and oceans consumes three hours of CRAY Y-MP time for each simulated year. Since the onset of an Ice Age takes about 10,000 years, "that's 30,000 simulation hours," says UIUC Atmospheric Sciences Professor **Michael Schlesinger**. "Obviously, that's a little impractical."

Instead, Schlesinger and Research Programmer **Ayman Ghanem** use the complete model to simulate the climate only at the beginning of the cycle. Then **Mikhail Verbitsky**, a research scientist in the geology and geophysics department at Yale University, inputs this information to a computationally less-demanding model that calculates the location and thickness of ice sheets and the displacement of the Earth's upper crust.

These simulations are the first to successfully demonstrate that orbital changes can lead to growth of the ice sheets. Schlesinger says that "we are carefully checking our calculations, because there are physical processes going on that cannot be resolved in the model due to computational limitations of current supercomputers."

Nonetheless, this success offers some assurance that Schlesinger's climate model can address the current question of global warming.

"How can we gain confidence that what we are predicting for the future is correct?" asks Schlesinger. "The only way to do this is to see how the models simulate past climates."

For a doubling of carbon dioxide (CO_2) in the Earth's atmosphere, Schlesinger's model predicts a rise in temperature of about 4 degrees Celsius, leading to a rise in sea level of about one meter over the next couple of centuries. ▲

CAUTION SIGNS ON THE INFORMATION SUPERHIGHWAY

BY PAULETTE SANCKEN, NCSA PUBLIC INFORMATION SPECIALIST

As an editor and writer in the world of technology, I've been hearing about and using the terms associated with the electronic—or information—superhighway for some time. I confess to being weary of the clichéd terms and analogies associated with driving that this technology has spawned. But I realize that for many, these terms and concepts are still quite new and exciting. For those unfamiliar with cyberspace, perhaps Howard Rheingold's *The Virtual Community: Homesteading on the Electronic Frontier* will act as a guide through "the wildly varied assortment of new cultures that have evolved in the world's computer networks over the past ten years."

Author of five books and numerous columns, Rheingold is editor of the San Francisco-based *Whole Earth Review*, a publication from the late 1960s. During that period, what was known as the *Whole Earth Catalog* was more interested in saving the world than technology. Now Rheingold is of the opinion that technology will transform civilization.

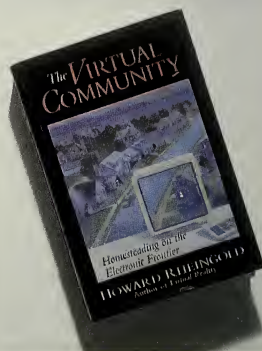
In the introductory chapter, Rheingold states "I have written this book to help inform a wider population about the potential importance of cyberspace to political liberties and the ways virtual communities are likely to change our experience of the real world as individuals and communities. Although I am enthusiastic about the liberating potential of computer-mediated communications, I try to keep my eyes open for the pitfalls of mixing technology and human relationships. I hope my reports from the outposts and headquarters of this new kind of social habitation,

and the stories of the people I've met in cyberspace, will bring to life the cultural, political, and ethical implications of virtual communities both for my fellow explorers of cyberspace and for those who never heard of it before."

Rheingold devotes much of the book to sharing his experiences as a participant in the WELL (Whole Earth 'Lectronic Link), a West Coast online coffee klatch. This virtual community is a group of people who thrive on spending time together in cyberspace discussing current events, soliciting help with personal problems, debating the latest net newcomer's idiocy, conducting business, and playing games. Apparently this activity has consumed vast amounts of time for many of the WELLbeings.

Aside from descriptions of everyday life on the Net, he also explores the reasons why so many people find spending time online so tempting. Rheingold wonders whether cyberspace is "precisely the wrong place to look for the rebirth of community, offering not a tool for conviviality but a life-denying simulacrum of real passion and true commitment to one another."

Further on he asks: "If a lonely person chooses to spend many hours a day in an imaginary society, typing witticisms with strangers on other continents, is that good or bad?"



(Photo by Film Processing Ltd.)

The Virtual Community may entice Net novices to get connected to online services to discover what all the commotion is about. It may also spur the extant online community to begin the process of protecting this source of freedom of speech. Perhaps the biggest eye-opener is that most people on the Internet are using it to meet others and maintain online relationships, not to get the latest information on the weather in Maui or how their senator voted on the last bill.

An extensive bibliography, approximately six pages long, on many aspects of Net connections adds value to this book.

Published by Addison-Wesley Publishing Co. ISBN 0-201-60870-7. Hardcover: \$22.95. ▲

abbreviations

ARPA	Advanced Research Projects Agency
CTC	Cornell Theory Center
DoE	Department of Energy
HPCC	High Performance Computing and Communications
NASA	National Aeronautics and Space Administration
NCAR	National Center for Atmospheric Research
NCSA	National Center for Supercomputing Applications
NII	National Information Infrastructure
NSF	National Science Foundation
PSC	Pittsburgh Supercomputing Center
SDG	Software Development Group
SDSC	San Diego Supercomputer Center
SGI	Silicon Graphics Inc.
TMC	Thinking Machines Corp.
UIC	University of Illinois at Chicago
UIUC	University of Illinois at Urbana-Champaign
URL	Uniform Resource Locator
VEG	Virtual Environments Group
WWW	World Wide Web

documentation orders

Articles in this *access* may refer to items that are available through the *NCSA Technical Resources Catalog*. To receive a copy of the catalog, send your request to Orders for Publications, NCSA Software, and Multimedia [see *nscsa contacts*, page 2].

accessing NCSA's servers

Many NCSA publications (e.g., calendar of events, user guides, *access*, technical reports) as well as software are available via the Internet on one of three NCSA servers: anonymous FTP, Gopher, or the World Wide Web. If you are connected to the Internet, we encourage you to take advantage of the easy-to-use servers to copy or view files.

Anonymous FTP IP address: `ftp.ncsa.uiuc.edu` (141.142.20.50)

Gopher server IP address: `gopher.ncsa.uiuc.edu`

World Wide Web IP address: `www.ncsa.uiuc.edu`

NCSA WWW Home Page: `http://www.ncsa.uiuc.edu/General/NCSAHome.html`

NOTE: References in *access* to a World Wide Web URL (Uniform Resource Locator) refer to the server address and file location information used by NCSA Mosaic software to retrieve documents.

If you have any questions about accessing the servers, contact your local system administrator or network expert. Instructions for accessing the anonymous FTP server follow.

downloading from anonymous FTP server

A number of NCSA publications are installed on the NCSA anonymous FTP server. If you are connected to Internet, you can download NCSA publications by following the procedures below. If you have any questions regarding the connection or procedure, consult your local system administrator or network expert.

1. Log on to a host at your site that is connected to Internet and running software supporting the FTP command.
2. Invoke FTP by entering the Internet address of the server: `ftp ftp.ncsa.uiuc.edu` or `ftp 141.142.20.50`
3. Log on using `anonymous` for the name.
4. Enter your local login name and address (e.g., `smith@ncsa.uiuc.edu`) for the password.
5. Enter `get README.FIRST` to transfer the instructions file (ASCII) to your local host.
6. Enter `quit` to exit FTP and return to your local host.
7. The NCSA publications are located in the `/ncsapubs` directory.

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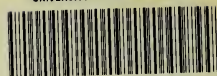


access

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